Exploring Earth and Planetary Materials with Neutrons

DAVID R. COLE and NANCY L. ROSS, Guest Editors

Neutrons “101” – A Primer

Where’s the Hydrogen?

Nanoscale Structure and Dynamics

Melts, Glasses, and Amorphous Materials

Phase Transitions and Magnetism

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Exploring Earth and Planetary Materials with Neutrons

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WHAT HAVE NEUTRONS EVER DONE FOR US?
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Upstairs in a secret and secure location, mineralogical activists have gathered…

RICH: Alright everyone, settle down. I hereby call this extraordinary meeting of the Society for the Protection of Analytical Methods [SPAM] to order. Brothers and sisters, we face a grave threat. For decades, we’ve provided X-rays and electrons to study the structure and properties of natural materials — everything a mineralologist could ever dream of. But now this!

[Frantically waves the “Exploring Earth and Planetary Materials with Neutrons” issue of Elements.]

They are threatening to take it all away from us! They’ve bled us dry! They’ve taken everything we had, and not just from us, but from our fathers, and from our fathers’ fathers.

NANCY: And from our fathers’ fathers’ fathers.

RICH: Yeah. All right. I’ll grant you hydrogen and magnetism are two things that neutrons can do pretty well.

[First laugh of the meeting.]

NANCY AND JODI: Oh, yes!

RICH: And apart from the hydrogen, the magnetism, and vibrational spectroscopy.

JODI: And the vibrational spectroscopy.

RICH: Well, yeah, obviously, the vibrational spectroscopy. I mean, that goes without saying, doesn’t it? But apart from the hydrogen, the magnetism, and vibrational spectroscopy...

DAVID: Isotopic substitution!

NANCY: Neutron activation analysis!

JODI: Total scattering!

RICH: Yeah, yeah. All right. Fair enough.

DAVID: All those disordered structures...

NANCY and JODI: Oh, yes!

DAVID: Yeah. Yeah, that’s something we’d really struggle with without neutrons.

NANCY: Small angle scattering, tomography of nanoporous structures!

JODI: And we can make complex sample environments, Rich.

DAVID: Yeah, given how weakly neutrons interact with matter, let’s face it, they’re the only ones who could get through some of the high-pressure rigs we have in a place like this.

ALL: Heh heh heh.

RICH: All right, all right. But apart from hydrogen, magnetism, lattice dynamics, isotopic substitution, chemical imaging, disordered structures, 3-D imaging, and the ability to build complex sample environments, I ask you: what have neutrons ever done for us?

NANCY: Hydrogen?

RICH: Total scattering.

NANCY: Isotopic substitution.

RICH: And magnetism.

NANCY: Oh, yeah, the magnetism Rich! Remember what it used to be like trying to determine magnetic structures...

RICH: Oh. Yeah, yeah. They do do that I suppose, yeah.

JODI: And magnetism.

NANCY: Oh, yeah, the magnetism Rich! Remember what it used to be like trying to determine magnetic structures?

RICH: Yeah. All right. I’ll grant you hydrogen and magnetism are two things that neutrons can do pretty well.

Richard Harrison
Principal Editor
ABOUT THIS ISSUE

In just about every physical science course the concept of the atom is taught. Students are introduced to the three subatomic particles of electrons, protons, and neutrons. Usually, there is a lot of emphasis on electrons, because their configuration determines the chemical properties of an atom. And the protons get a lot of attention as well: who doesn’t like H+? Sadly, too often, neutrons are left in the “Oh, there is another part of an atom” category … that neutral subatomic particle that adds weight to the atom.

The neutron was discovered in 1932, several decades after the discovery of the electron and the proton. But, the neutron took the world by storm in the 1930s with the discovery of nuclear fission in 1938 and the birth of the atomic age. Many of us benefit from neutrons, because they are the backbone of the nuclear power industry. And, with the advent of dedicated neutron sources such as neutron generators and spallation sources, we also benefit from neutrons as the basis for experiments such as those featured in this issue of Elements. Nancy Ross and David Cole open their introductory article with the statement, “The fundamental properties of the neutron make it a powerful tool for Earth science investigations because neutrons provide information that cannot be obtain by any other research method.”

We hope that after reading the articles in this issue of Elements that the neutron will move from the “Oh, there is another part of the atom” category to “Wow! Let me tell you about the neutron” category.

VISIBILITY OF ELEMENTS

The Clarivate™ Journal Citation Reports for 2020 were released in July 2021. Elements’ journal impact factor for 2020 was 3.671. For your reference, the journal impact factor takes into consideration the citation rate of only those articles published in the previous 2 years: in this case, those published in 2018 and 2019 and cited in 2020. Elements’ journal impact factor (JIF) has remained relatively steady over the past 10 years (see graphic).

The 585 thematic articles published in Elements from 2005 to 2020 have received a total of 26,935 citations. Elements articles have been cited in 2,833 different journals. Approximately a third of those citations are found in the 15 journals shown in the graphic below, with the journals Geochimica et Cosmochimica Acta, Lithos, Chemical Geology, Earth and Planetary Science Letters, and Ore Geology Reviews being most popular.

In our June 2018 issue (v14n3), we highlighted that there were four Elements articles that each had over 200 citations. Three years later, the number of 200+ citation articles has almost quadrupled (15 articles). And, at the time of the release of this issue, there are 5 articles that have well over 400 citations each. Three of these articles were on our 2018 list, but there are two articles on zircons that have recently found popularity in the literature, and they now join the 400+ club.

- “Water Management Challenges Associated with the Production of Shale Gas by Hydraulic Fracturing” by Gregory et al. (2011, v7n3, pp 181–186) – 526 citations
- “Re-equilibration of zircon in aqueous fluids and melts” by Geilser et al. (2007, v3n1, pp 43–50) – 522 citations

Each Elements issue contains 5–7 thematic articles that collectively present a coherent picture of a topic. So, even though we celebrate the successes of individual articles, such as those listed above, we believe that it is also important to evaluate the collective impact of our thematic issues. As of July 2020, 48% of the 95 Elements issues have had over 200 citations each, with the most highly cited issues since the time of publication being the following:

- v3n1 – “Zircon, Tiny but Timely” (1,670)
- v8n5 – “Rare Earth Elements” (1,016)
- v4n5 – “CO2 Sequestration” (970)
- v10n2 – “Ophiolites” (957)
- v7n2 – “Iron in Earth Surface Systems” (859)
- v2n2 – “Arsenic” (798)
- v3n5 – “The Critical Zone” (765)
- v4n2 – “Phosphates and Global Sustainability” (733)

Some of these issues continue to receive ~150+ new citations a year, even though they were published almost 10 years ago. This is evidence of the staying power of Elements.

We can confidently say that Elements’ readers have access (in print and online) to excellent articles on relevant topics that have lasting interest to our scientific community.

BREAKING NEWS

Janne Blicher-Toft has accepted our invitation to join the editorial board of Elements. Beginning in January 2022, she will assume the role of Principal Editor – Geochemistry. Janne is a research director with the CNRS at the École Normale Supérieure de Lyon (France). She is a geochemist who specializes in radiogenic and stable isotopes with applications to geochronology, terrestrial and planetary mantle–crust evolution and mantle dynamics, mantle geochemistry, crustal growth, early Earth geodynamics, early life, planetology, cosmochronology, meteoritics, anthropology, geoaarheology, archaeology, and numismatics. In addition to her research activities, she serves as an editor for several geochemical journals including Geochimica et Cosmochimica Acta; Geochemistry, Geophysics, Geosystems; and Geochemical Perspectives. We look forward to working with Janne in the years ahead.

John Eiler, Richard Harrison, Becky Lange, and Jodi Rosso
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SERVING THE GLOBAL GEOANALYTICAL COMMUNITY
DIVERSITY AMONG EDITORIAL BOARDS OF ELEMENTS AND OTHER SELECTED GEOCHEMISTRY, COSMOCHEMISTRY, MINERALOGY AND PETROLOGY JOURNALS

Olivier Pourret1,*, Jennifer L. Middleton2, Daniel E. Ibarra3,4, Dasapta Erwin Irawan5, Ashaki Rouff6, Pallavi Anand7, Aradhna Tripati8, Amy J. V. Riches9,10, and Anthony Dosseto11

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The publication of scientific work is foundational to our disciplines. To ensure equitable publication standards during the global flow of knowledge production, professional societies and publishers must take positive steps to avoid biases that might hinder the publication of scientific work (see Liévano-Latorre et al. 2020). Biases among editors and reviewers can be unconscious and be influenced by different aspects of an author’s identity: country of origin, first language, affiliation, gender identity, ethnicity, and/or other factors. These biases could result in challenges to publication rates and visibility in key journal forums for under-represented groups (Lerback et al. 2020). Ensuring that there is diversity in the peer review and publishing process, and on editorial boards, may help to eliminate bias.

Diversity promotes innovation from hypothesis through peer review to final publication (e.g., Hofstra et al. 2020) and should be set as a new standard, as shown by the Royal Society of Chemistry (https://www.rsc.org/new-perspectives/talent/joint-commitment-for-action-inclusion-and-diversity-in-publishing/). Personal identity has an impact on how we engage with our science; it impacts how we approach a problem, and what we value, study, and write. It influences how we select reviewers, how we review, and, ultimately, what is successfully published. Therefore, the limited diversity of major editorial boards will act as a barrier to representation of all academic members. The members of editorial boards shape the direction and success of a journal, and they influence the authorship of papers and what is published within the journal. Differences in scientific networks may be a core reason for the persistence of implicit bias from editorial boards, particularly with regard to gender (Hanson et al. 2020). Therefore, editorial bias, or perceived editorial bias, can exclude certain groups and exacerbate historical inequities regarding under-representation of entire continents within the geoscience literature (e.g., Africa, see North et al. 2020). Hence, for an editorial board to be inclusive and unbiased, it needs to be as diverse as the research community it represents, which we know does not exactly reflect the general population.

In this piece, we provide an exploration of diversity among editorial boards by presenting data for Elements in terms of gender and geographic affiliation. We further compare these data with editorial board data from journals that are published by the societies that jointly publish Elements (hereafter termed the “journals of the participating societies”).

Historically (from 2005 to 2021), 19 principal editors (PEs) have served with Elements: among them, four were women (21%). In the past 10 years, there have been 11 PEs, 3 of which have been women (27%). These numbers, though falling short of gender parity, are representative of the proportion of the mid- to late-career women in the field and are indicative of the wider challenges to diversity in our discipline. The executive editor is also considered part of the editorial board: both executive editors have been women. So, Elements’ editorial board (executive and principal editors) has always had 25%–50% women at any one time. All serving editors are white and are affiliated with institutions in Northern America (n = 13; 62%; USA and Canada) or Western Europe (n = 8; 38%; UK, France, Germany, Denmark).

In the first stage of our study, gender information was obtained from the editorial boards of Elements and the participating societies (see Table 1). Gender data were available for all editorial boards, except for the boards of Ecosphere and Geochemistry, Geophysics, and Geosystems’ Journal of Geophysical Research: Solid Earth. Of the 166 editorial board members, 30% (49) were women. Notably, almost all elected editorial board members were white, and 64% (106) of all editorial board members were affiliated with institutions in Northern America. The limited diversity of editorial boards is also reflected in the membership of editorial boards, where 87% (145) of all editorial board members were white; only 13% (21) were non-white, including 3% (5) that identified as Latina or Latina (see Table 1).

Figure 1. Gender breakdown of editorial board members from selected journals; data accessed on journal websites on 8 April 2021. Editorial board members were assigned a binary gender using first names and, in some cases, based upon the authors’ own perceptions and knowledge. Abbreviation: n = number of editorial board members. There are two notable limitations to this analysis: (i) it may misgender people; (ii) gender is not binary, and non-binary people were not included in this first-stage analysis due to lack of available information.
Examination of the editorial team among the journals of the participating societies highlights the pervasiveness of a lack of editorial diversity within our field (17 journals published and edited by various commercial publishers and learned societies) (Fig. 1). Here, we identify that, as of April 2021, the current editorial boards span a range of gender representation from 7 (50%) men and 7 (50%) women for Geochemical Perspectives Letters to 37 (97%) men and 1 (3%) women for the Journal of Mineralogical and Petrological Sciences. Of the 683 editorial board members in total, 142 (21%) are women and 539 (79%) are men. These numbers are comparable to the February 2021 Elsevier Benchmark Gender Diversity distribution of portfolio editors across the fields that Elsevier term “Geochemistry & Planetary Science” (25% women, 74% men and 1% preferred not to disclose) and “Applied Geosciences” (14% women, 86% men). It must be noted that numbers from Elsevier are from an incomplete voluntary survey of the editors, yet these do provide a good indication of gender distribution. Moreover, in some of the journals (i.e., those with larger editorial boards), turnover happens more quickly and, thus, numbers can fluctuate up to a few percent in six months.

As with gender distribution, geographic distribution is also strongly biased (Fig. 2). A given country is based on the affiliation of editors and implicitly may create a bias when an editor originates from one country and moves to another country. Journals such as Chemical Geology (36% from Northern America, 41% from Western Europe, 2% from Sub-Saharan Africa, 2% from Northern Africa and Western Asia, 2% from Central and Southern Asia, 5% from Eastern and South-Eastern Asia, and 12% from Oceania) and Geochemistry: Exploration, Environment, Analysis (14% from Northern America, 10% from Latin America and the Caribbean, 38% from Western Europe, 10% from Eastern Europe, 5% from Sub-Saharan Africa, 10% from Eastern and South-Eastern Asia, and 14% from Oceania)HER) are the more geographically diverse, whereas Elements (75% from USA and 25% from Western Europe), Journal of Mineralogical and Petrological Sciences (79% from Japan) and Swiss Journal of Geosciences (79% from Switzerland) are more limited in geographic representation among editors. Such differences, in spite of ongoing efforts by participating societies to progress scientific excellence via improved diversity and inclusion, may be explained by unconscious bias arising from legacy influences and the current management of expectations for editorial roles. Most journals are published in English and editors are expected to be native or fluent in English; therefore, most editorial boards would consist of individuals who originate from countries where English is an official language (e.g., United Kingdom, United States). Moreover, the regional scope of some journals, such as the Swiss Journal of Geosciences (readership from Switzerland) and Journal of Mineralogical and Petrological Sciences (readership from Japan), can also explain a distribution biased towards a specific region.

Overall, editorial board members are predominantly from Western Europe (39%), Northern America (29%), Eastern and South-Eastern Asia (16%), and Oceania (5%). If we look at gender distribution among regional groupings, Latin America and Caribbean editorial board members are 46% women and 54% men (but represent less than 2% of the total), whereas Northern America and Western Europe have a distribution of 23%–77% women and 26%–74% men. Eastern and South-Eastern Asia distribution is far less balanced: 5% women and 95% men. The observed differences in gender distribution likely reflect regional or local progress towards gender equality (Hori 2020).

The results presented in this Triple Point show that there is a persistent diversity imbalance in editorial boards compared to the research community as a whole, something that was identified more than a decade ago by Mukasa (2009). This inequitable representation is being exacerbated because our community demographics do not demonstrate gender or racial parity (Bernard and Cooperdock 2018; Pourret et al. 2021) and women are also under-represented as first authors relative to their representation in the field of geoscience (Pico et al. 2020). Scientific excellence may suffer as a consequence of this imbalance. There needs to be more women and under-represented groups in the field (which is happening, albeit slowly), and there needs to be an equity lens used for assigning workloads (rewards and professional progression) that reflects different service loads. Otherwise, it is inevitable that early career, mid-career, and senior scientists from under-represented groups will have to carry unduly heavy workloads in order to fill the diversity needs of committees and editorial boards. It is not uncommon for invitations to serve on an editorial board to be rejected by women and scientists of under-represented groups because they are already too busy with other service activities that may provide more immediate community and professional benefit.

To improve scientific excellence and diversity, journals could implement the following:

1. Set up a diversity working group that can help identify potentially qualified editorial board members and editors-in-chief, while also targeting an increase in diversity.

2. Editors-in-chief may invite identified people (see point 1) to join their editorial board when a position is available (no necessity of expansion, but growth may accelerate the changes). They should emphasise their results and efforts toward diversity/equity/inclusion at the journal’s society meetings and in doing so educate members about editorship diversity.

**Figure 2** Geographical distribution of editorial board members by journal, with regional groupings based on indicators of sustainable development goals; data accessed from journal websites on 8 April 2021. Editorial board members were assigned a region using the country of their affiliation. Abbreviation: n = number of editorial board members.
A BRIEF HISTORY OF MINERAL SYMBOLS

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Laurence N. Warr

At some stage you may have abbreviated the name of a mineral when writing a thesis, report, or publication. This could have been for a common mineral such as quartz (Qz) or muscovite (Ms). But there are some more notoriously long mineral names for which a shortened version can be rather useful. Take, for example, the 34-letter-long potassic-magnesio-fuuro-arfvedsonite (usefully abbreviated to “Pmfarf”, where “arf” represents “arfvesonite”). Our friends the chemists long ago got their act together and developed a universally accepted system for abbreviating the chemical elements in a system that uses either one or two letters as symbols. This scheme was first proposed by chemist Jöns Jacob Berzelius (1779–1848) and is still applied over 200 years later under the auspices of the International Union of Pure and Applied Chemistry.

So, what about minerals? Adopting the very same idea of using letter symbols as abbreviations, Ralph Kretz (University of Ottawa, Canada) presented a pioneering short paper in 1983 entitled “Symbols for rock-forming minerals”. Known as Kretz symbols, he used two- or three-letter symbols to represent 192 of the more common mineral species. This list was later modified and updated to 371 minerals by Whitney and Evans (2010), which today has become the more widely applied set of abbreviations.

However, the buck didn’t stop here. Because available abbreviation listings are recommendations rather than rules, there has been a bit of a free-for-all in abbreviation use by the mineral community. According to a survey of published clay mineral abbreviations conducted in 2020 (Warr 2020), only 30% of authors used the recommended Kretz symbol for kaolinite (“Kln”). For this mineral, and for many other common species, there were no less than 8 different symbols in use for the same name. And what about the many minerals that have not been allocated a recommended abbreviation? Currently, there are over 5,700 approved minerals but less than 18% have been included in any published list of symbols.

For fun: there are 30 natural elements listed as minerals. Can you work out which ones?

Happy symbolizing.

Laurence N. Warr

(University of Greifswald, Germany)

REFERENCES


MINERAL MATTERS

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(3) Individual editorial board members may give personal encouragement, and act as mentors, to potential editors who are of diverse backgrounds and identities.

(4) Ask scientists from under-represented groups how they could be supported in order to participate on an editorial board, for example through workloads that are set using principles of equity.

(5) Journals editorial boards present an infographic of diversity of the editorial board and/or the geographical scope of the published articles. This may attract attention from diverse researchers, as well as raise awareness of diversity/equity/inclusion in the scientific publishing space.

One-time actions to tackle diversity are not enough. Journals must monitor the impact of new diversity efforts to ensure real change is happening on their boards.

Recent shifts towards more equal gender and geographic representation for Elements, Geochemical Perspectives Letters or Geochemica et Cosmochimica Acta are very encouraging, but this is not the case for all the journals from the participating societies. Achieving representative diversity on editorial boards needs sustained effort. Furthermore, we recommend that the editorial boards of the journals published by Elements participating societies should consider prioritizing and establishing a mentoring approach to address negative and unconstructive critiques of articles. Finally, the barriers to publishing must be minimized. This is particularly important given the unequal impacts of the COVID-19 pandemic on submissions by men and women and their geographical location of origin.

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Gilberto Artioli is a professor of mineralogy, crystallography, and materials science at the University of Padova (Italy). He received a Laurea Degree from the University of Modena (Italy) and a PhD from the University of Chicago (Illinois, USA). His interests focus on mineralogy and industrial materials. His scientific expertise encompasses the use of combined techniques, including those based at large-scale facilities, for the investigation of complex materials. He is the Director of the Interdepartmental Centre of Research and Study of Cements and Hydraulic Binders at the University of Padova and the Chair of the International Union of Crystallography’s Commission on Crystallography in Art and Cultural Heritage.

Chris J. Benmore is a physicist at the Argonne National Laboratory (Illinois, USA) and, since 2008, has been an adjunct professor at Arizona State University (USA). He obtained his PhD from the University of East Anglia (UK). His postdoctoral work was at the University of Guelph (Canada) and the neutron scattering center at Los Alamos (New Mexico, USA). He was a neutron instrument scientist at the ISIS facility of the Rutherford Appleton Laboratory (UK) and at the Intense Pulsed Neutron Source at the Argonne National Laboratory. His work focuses on glasses, liquids, and amorphous materials, with an emphasis on structures at extreme conditions. In 2012, he was awarded the University of Chicago Medal for sustained research.

Bryan C. Chakoumakos is a Corporate Fellow at the Oak Ridge National Laboratory (ORNL) (Tennessee, USA) where he conducts research on novel and technologically important materials. He employs crystallography and neutron/X-ray diffraction methods, publishing broadly in physics, materials science, chemistry, and mineralogy. He received his PhD in geological sciences from Virginia Tech (USA) in 1984, working with Gerry Gibbs, and did a postdoctoral fellowship at the University of New Mexico (USA) working with Rod Ewing. He joined ORNL in 1987 working with Lynn Boatner. In 1993, his primary focus shifted to neutron scattering. He now manages the Single-Crystal Neutron Diffraction Group, which operates five neutron diffractometers, at the High Flux Isotope Reactor and the Spallation Neutron Source at ORNL, which is a DOE Office of Science user facility.

David R. Cole is Professor, Ohio Research Scholar, and Endowed Chair in Subsurface Science and Sustainability at the School of Earth Sciences at Ohio State University (OSU) (USA). He obtained his PhD in geochemistry and mineralogy from Pennsylvania State University (USA). He is a faculty advisory board member of the OSU Sustainability Institute (SI), and co-lead for the Sustainable Energy Research section of the SI. Prior to coming to OSU in 2010, he was a distinguished scientist and head of the Geochemistry and Interfacial Sciences Group in the Chemistry Division of Oak Ridge National Laboratory (Tennessee, USA). His current research focuses on interrogating the mechanisms, rates, and the transport behavior associated with energy-relevant water–gas–mineral (rock) interactions using advanced electron microscopy, nuclear magnetic resonance spectroscopy, neutron scattering, X-ray computed tomography, and molecular dynamics. He is a Fellow of the Mineralogical Society of America and of the Geological Society of America.

G. Diego Gatta is professor of applied mineralogy at the University of Milan (Italy). After completing his PhD at the University of Perugia (Italy), he worked as a postdoc at the Bayerisches Geoinstitut, Bayreuth (Germany) before moving to the University of Milan in 2005. He was the recipient of the Max Hey Medal of the Mineralogical Society of Great Britain and Ireland in 2008, was awarded the European Mineralogical Union Medal in 2013, and has served as President of the Italian Crystallographic Association. His diverse areas of research include the structure–property relationships of minerals and their synthetic counterparts (order–disorder processes, equations of state, and phase transitions); detecting protons and structurally incorporated guest molecules in open-framework materials; and industrial and technical mineralogy (environmental and forensic mineralogy, ceramics, gemmology).

Klaudia Hradil is head of the X-ray Center at the Vienna University of Technology (Technical University of Vienna) (Austria). The X-ray Center solves problems in materials research and is a center for developing new X-ray methodologies. Klaudia studied mineralogy/crystallography at the Ludwig Maximilian University of Munich (Germany) and obtained her PhD there on the subject of disorder and superorder scattering phenomena. She has a 30 years’ experience in X-ray and neutron scattering techniques and instrumentation.

Daniel S. Hussey is a physicist at the National Institute of Standards and Technology (NIST) (Maryland, USA) where he leads a team in the development of novel neutron imaging and optics techniques. He works to improve spatial resolution by developing new detectors and imaging methods, notably an analog to Hooke’s microscope using Wolter optic mirrors. One exciting new research project under development is the NIST INFER project that will provide multiscale images. He holds one patent, coauthored over 180 papers, is a Fellow of the American Physical Society, and has received the Presidential Early Career Award for Scientist and Engineers, the Arthur S. Flemming Award, and an R&D 100 Award.

Martin Meven is group leader and instrument scientist of the HEIDi single crystal diffractometer operated jointly by the RWTH Aachen University and the Jülich Centre for Neutron Science of the Forschungszentrum Jülich at the neutron source FRM II of the Heinz Maier-Leibnitz Zentrum (MLZ) in Germany. Martin obtained his PhD in crystallography at RWTH. He developed a new high-resolution X-ray single crystal diffractometer and studied the local disorder of ceramic superconductors by neutron diffraction, for which he was awarded the Friedrich-Wilhelm Prize. Since 2001, he has worked at MLZ where he has developed the HEIDi instrument to study framework and disordered structures, and where he develops new methodologies. He is spokesman of the neutron scattering work group of the German Society of Crystallography.

Cont’d on page 154
John B. Parise is SUNY Distinguished Professor in Geosciences and Chemistry at Stony Brook University (New York, USA). He directs GENESIS (a next generation synthesis center) at one of the Department of Energy’s Energy Frontier Research Centers, and is the Director of the Stony Brook University’s Photon Sciences Institute. He obtained his PhD from James Cook University (Australia) for research carried out while in residence at the Australian Atomic Energy Commission’s research reactor at Lucas Heights. He has a background in crystallography, geochemistry, and inorganic synthesis. His research is on the formation, evolution, and atomic arrangements in nano- and amorphous phases formed via liquid-mediated and high-pressure synthesis.

Nancy L. Ross is a professor in the Department of Geosciences at Virginia Tech (USA). She earned her MS from the University of British Columbia (Canada) and her PhD from Arizona State University (USA). Prior to joining Virginia Tech in 2000, Nancy was a Reader in the Department of Geological Sciences at University College London (UK). She uses neutron diffraction and inelastic neutron scattering to study the structure and dynamics of materials. She has served as President of the Mineralogical Society of America (2009) and as Principal Editor of Elements (2017–2020). She is a member of Neutron Advisory Board (NAB) for Oak Ridge National Laboratory (ORNL) and is a member of the Second Target Station Project Advisory Board for ORNL. Nancy is also a Fellow of the Mineralogical Society of America and of the Geological Society of America, and she is an Honorary Fellow of the Società di Mineralogia e Petrologia.

Andrew G. Stack is a geochemist who is Group Leader and Interim Director of the Chemical Sciences Division at Oak Ridge National Laboratory (Tennessee, USA). He focuses on understanding reaction mechanisms and rates of mineral–water interfaces in aqueous solutions, with the goal of improving our ability to predict the rates of geochemical phenomena that occur in porous media, processes that are themselves important to society. To understand structure, dynamics, and reactivity, he often combines microscopy with in situ X-ray/neutron scattering experiments and with atomic-scale computational simulations.

Hsiu-Wen Wang is research scientist in the Geochemistry and Interfacial Science Group, Chemical Sciences Division, Oak Ridge National Laboratory (Tennessee, USA). She did a postdoctorate in neutron scattering at Oak Ridge and at the Los Alamos National Laboratories (2011–2014) and a PhD and an MS in mineralogy/geochemistry from Indiana University (USA) (2005–2011). She established herself as an expert in total scattering techniques and has contributed new insights to coordination and local order in both homogeneous and heterogeneous materials. She is interested in molecular-based interpretations of scattering results, and, using advances in structural characterization, offers insight into how complex functional materials work, both at the bulk scale and the nano-scale.

Martin C. Wilding received his PhD from the University of Edinburgh (UK) where he studied mineral inclusions in natural diamonds. Subsequently, he focused on the thermodynamics and structure of amorphous materials and liquids: this he did while working at the University of Bayreuth (Germany) and with Alexandra Navrotsky’s group at the University of California Davis (USA). He has worked at both pulsed and reactor neutron sources to study liquids and amorphous materials under extreme conditions, and has used quasi-elastic neutron scattering to determine the diffusion of sodium ions in molten carbonate and nitrate. Martin has also used neutron diffraction with isotopic substitution (NDIS) to investigate the restructuring of solvents surrounding carbon nitride and graphene oxide nanoparticles. Most recently, he has used NDIS to study the changes in liquid structure during the invert crystallization of organometallic hybrid perovskites. Currently, he works as an experimental officer at the UK Catalysis Hub.

Excalibur Mineral Corp.
1885 Seminole Trail, Ste 202, Charlottesville, VA 22901-1160, USA
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Neutrons “101” – A Primer for Earth Scientists

Nancy L. Ross1 and David R. Cole2

INTRODUCTION

The neutron can be used as an amazingly diverse probe by which to investigate Earth materials. The neutron particle was discovered in 1932 by British physicist James Chadwick (Chadwick 1932) and, from that moment, started the development of neutron diffraction and spectroscopic techniques. In the 1940s and 1950s, nuclear reactors, as sources for neutrons, became available to researchers shortly after World War II. Two of the leaders in this emerging field of research, Professor Bertram N. Brockhouse (McMaster University, Canada) and Professor Clifford G. Shull (Massachusetts Institute of Technology, USA), were awarded the 1994 Nobel Prize in Physics for their pioneering contributions to the development of neutron scattering techniques, as well as their studies of condensed matter and developing the neutron diffraction technique. In simple terms, they helped answer the questions of where atoms “are” and what atoms “do”. Since then, neutron scattering techniques have played an important role in investigating the atomic-scale origins of a material’s structure, as well as its physical, electrical, and magnetic properties. To date, however, relatively few researchers in the Earth sciences are taking advantage of the unique opportunities provided by neutron facilities. As the articles in this issue illustrate, the interaction of neutrons with Earth materials provides unique opportunities for researchers in the fields of mineralogy, geochemistry, and petrology. Neutrons provide a valuable means of exploring such geologic processes as subduction, earthquake generation, and volcanic eruptions, all of which depend on the physical, chemical, and rheological properties of the materials involved. These, in turn, depend on the structure and properties of the constituent minerals and the associated hydrous components, which can be determined using the neutron techniques described in this issue.

Most of us are familiar with the various X-ray methods used for the detailed study of Earth materials. However, X-ray methods are not always adequate to fully characterize a material’s structural properties and dynamic processes. Unlike X-rays, which interact strongly with a material’s electrons, neutrons scatter from a material’s nuclei. The neutron’s fundamental attributes make it a unique and complementary probe to X-ray scattering and other techniques.

The purpose of this issue of Elements is to provide an introduction for those not familiar with neutrons and their broad-ranging applications. In this article, we introduce neutron science, starting with how the properties of neutrons make them such a unique probe, followed by how we produce neutrons and the major neutron sources where we can do a neutron experiment, followed by an overview of different types of neutron experiments that can be performed and the scientific opportunities, especially for the future. The other articles in this issue provide more in-depth examples of applying neutron scattering methods to the Earth sciences. For additional background, the reader is referred to Liang et al. (2009) and Wenk (2006a, 2012).

WHY NEUTRONS?

The neutron is a subatomic particle: it has zero charge, a mass of 1.0087 atomic mass units, a spin of 1/2, and a magnetic moment. These four properties combine to make neutrons a highly effective probe, providing unique opportunities for research on materials. Similar to X-rays, thermal neutrons have wavelengths comparable to interatomic distances in materials, so neutron diffraction can be used to study the structures of materials. Unlike X-rays, neutrons are scattered from the nuclei of atoms rather than the electron cloud, and neutrons have a strength indicated by a neutron scattering length ($b$) and a corresponding “cross section” ($\sigma$, which is the likelihood of the incident neutron interacting with a target nucleus) that varies from...
Neutrons can locate light atoms in the presence of heavy atoms. In contrast to X-rays, in which scattering is proportional to the number of electrons in the atom, the scattering from neutrons varies in a way that depends on the nuclear structure. The interaction of the spin of the neutron with the spin state of the nucleus of a given atom determines the scattering property of a neutron with that atom. This spin–spin interaction leads both to coherent scattering and to incoherent scattering (Squires 2012). Neutrons have a nuclear spin, making them very sensitive to hydrogen atoms.

A full list of neutron scattering lengths and thermal cross sections can be found in *Neutron News* (1992), which is easily accessed through the National Institute of Standards and Technology (NIST) website https://www.ncnr.nist.gov/resources/n-lengths/. The widely varying neutron scattering lengths among elements and their isotopes create a number of opportunities in the study of materials:

- Neutrons are particularly sensitive to hydrogen atoms. The pronounced neutron scattering cross section of hydrogen means that neutrons can be used to precisely locate hydrogen atoms and elucidate details of hydrogen bonding (e.g., Gatta et al. 2021 this issue).
- Neutrons can distinguish between different isotopes. Hydrogen (^1H) and deuterium (D = ^2H), for example, have widely different scattering lengths of ~3.739 fm and (~6.671 fm, respectively. The negative sign means that the scattered neutrons’ wave function is out of phase with respect to the incident neutrons.
- Neutrons can locate light atoms in the presence of heavy atoms (compare O and U in Fig. 1) and, in some cases, can distinguish between elements with similar atomic numbers. Redfern et al. (1997), for example, used neutron diffraction to study Fe/Mn order–disorder in olivine at high temperature.

In addition to exploiting the advantages provided by scattering from nuclei, neutrons also offer several other advantages:

- Neutrons have no charge and so interact with atomic nuclei through the very short-range nuclear force (Squires 2012). Consequently, a neutron beam penetrates matter much more deeply than an X-ray or electron beam can. One of the applications of this property is revealing the 3-D mapping of stresses deep inside rocks (e.g., Darling et al. 2004) and the imaging of rocks and cultural heritage artifacts (Artioli and Hussey 2021 this issue).
- Neutrons have a nuclear spin, making them very sensitive to the location and orientation of magnetic moments in materials. Neutrons, thus, are the probe of choice for many studies of magnetism. They can be used to map magnetic structures and phase transitions, as described by Chakoumakos and Parise (2021 this issue).
- Neutrons can transfer momentum and energy to a sample, making it very useful for the study of fundamental vibrations (phonons) within materials which gives information on the strengths of chemical bonds and vibrational density of states. Unlike infrared or Raman spectroscopy, there are no selection rules for inelastic neutron scattering (Parker et al. 2011).
- Nuclei act as pinpoint scatterers compared to X-ray scattering in which the electron cloud has a size comparable to the wavelength of the probing radiation. Thus, the neutron scattering length, b, is independent of the scattering angle, which is in contrast to X-rays where the scattering decreases with increasing scattering angle. Thus, the smaller d-spacing between planes of atoms is better constrained in a neutron experiment as compared to a similar X-ray experiment.

**Table 1**

<table>
<thead>
<tr>
<th>Reactor Sources</th>
<th>Neutron Sources under Construction (*)</th>
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<tr>
<td>Opal Pool Australian Lighwater Reactor, Australian Centre for Neutron Scattering</td>
<td>(OPAL) ANSTO Lucas Heights (NSW, Australia)</td>
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<tr>
<td>Chalk River Laboratories, Canadian Nuclear Laboratories</td>
<td>CRL Chalk River (Canada)</td>
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<td>China Advanced Research Reactor</td>
<td>CARR Beijing (China)</td>
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<tr>
<td>Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research</td>
<td>FLNP Dubna (Russia)</td>
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<td>Forschungs-Neutronenquelle Heinz Maier-Leibnitz</td>
<td>FRM-II Munich (Germany)</td>
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<td>High Flux Isotope Reactor</td>
<td>HFIR Oak Ridge (Tennessee, USA)</td>
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<td>Institut Laue-Langevin</td>
<td>ILL Grenoble (France)</td>
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<td>Laboratoire Léon Brillouin</td>
<td>LLB Saclay (France)</td>
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<tr>
<td>Center for Neutron Research, National Institute for Standards and Technology</td>
<td>NIST Gaithersburg (Maryland, USA)</td>
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<td><strong>Spallation Sources</strong></td>
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<td>Chinese Spallation Neutron Source*</td>
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<td>European Spallation Source*</td>
<td>ESS Lundt (Sweden)</td>
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<tr>
<td>Rutherford-Appleton Laboratory</td>
<td>ISIS Harwell (Oxfordshire, UK)</td>
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<tr>
<td>Japan Proton Accelerator Research Complex</td>
<td>J-PARC Tokai (Japan)</td>
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<td>Los Alamos Neutron Science Center</td>
<td>LANSCE Los Alamos (New Mexico, USA)</td>
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<tr>
<td>Swiss Spallation Neutron Source, Paul Scherrer Institut</td>
<td>SINQ (PSI) Villigen (Switzerland)</td>
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<tr>
<td>Spallation Neutron Source</td>
<td>SNS Oak Ridge (Tennessee, USA)</td>
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**Figure 1** Comparison of coherent scattering lengths from X-rays and neutrons. The size of each circle is a measure of the relative cross section; mass numbers identify the different isotopes, with the top row representing an isotopically averaged value. Negative neutron scattering lengths are represented by blue circles. Modified after Kartini (2007).
Neutron scattering provides advantages over other methods because thermal/cold neutrons are a noninvasive probe that interacts only weakly with matter. Neutrons do not change the investigated sample because they do not deposit energy into it.

**NEUTRON PRODUCTION AND SOURCES**

Neutrons are bound in nuclei. This means that large energies are needed to liberate them. This is achieved either by nuclear fission in a reactor source or by spallation in a spallation source. Reactors deliver a continuous source of neutrons, whereas spallation sources deliver a pulsed beam. The neutrons so-produced have energies of tens or hundreds of MeV, which is far too high for investigations of condensed matter which requires neutrons to have much lower energies. Therefore, neutrons must be cooled to create a beam of “thermal” neutrons with energies around 25 MeV by passing the beam through a moderator (Squires 2012). The spectrum of neutrons emitted by a reactor is dependent on the moderator temperature. This spectrum is Maxwellian in shape and has a maximum that depends on the temperature. For example, for $T = 273$ K, $\lambda_{\max}$ (the maximum neutron wavelength) is around 1.55 Å; for $T = 373$ K, $\lambda_{\max}$ is 1.33 Å. Thermal neutrons have wavelengths that can be used to probe excitations across a range of length scales, through elastic and inelastic scattering processes as described below. Using “hot sources,” it is possible to move the maximum of the neutron spectrum to shorter wavelengths and, by cooling the moderator, the maximum of the neutron spectrum can be moved to longer wavelengths (Fig. 2). Because neutrons have no charge and cannot be focused, instruments at a neutron source are arranged around the moderators of the appropriate design.

In a reactor source, the thermal neutron is captured by a fissile heavy isotope, such as $^{235}$U, which typically splits into two lighter elements, plus 2 or 3 fast (high energy) neutrons, and a variety of light elementary particles (Fig. 2). This fission reaction is accompanied by a release of energy. A self-sustaining chain reaction requires one neutron per fission event to be scattered back into the fuel element and produce 1 or 2 neutrons per event. There are ~40 operational research reactors for neutron scattering around the world (https://nucleus.iaea.org) that are optimized for basic research experiments in addition to isotope production or fuel development. Examples of reactor sources can be found in Table 1. In a spallation source, a pulsed or quasicontinuous neutron beam is produced by accelerating protons to a target material of heavy nuclei, such as mercury, tantalum, or lead. Examples of spallation neutron sources are listed in Table 1. Generally, the production of neutrons at a spallation source begins with a high-powered proton accelerator: this could be a linear accelerator (“linac”) (e.g., SNS), or a combination of linac and synchrotron (e.g., ISIS), or a cyclotron (e.g., PSI). Protons hitting nuclei in the target material trigger an intranuclear cascade, placing individual nuclei into a highly excited state. The nuclei then release energy by evaporating nucleons (mainly neutrons), some of which will leave the target while others go on to trigger further reactions (Fig. 3). These neutrons are then slowed in moderators such as liquid hydrogen, liquid water, liquid methane, or solid methane to the energies that are needed for the scattering instruments. In contrast to the fission of heavy nuclides, one spallation reaction releases about 20–30 neutrons per incident particle, or ~10 times more than nuclear fission. Consequently, spallation has become an established technique for producing high-intensity fluxes of neutrons. However, the design of the targets for high-power spallation sources, having a beam power of several megawatts, presents a formidable technical challenge in terms of heat removal and of taking into account the radiation damage to the target and structural materials.

In comparison with X-ray sources, neutron sources have significantly lower fluxes and, therefore, larger amounts of sample are required for experiments. However, great advances have been made in increasing neutron flux since the days of the earliest neutron sources, which were based on radioactive decay. Their successors, the nuclear fission reactors, produced fluxes whose peak values reached a plateau in the 1950s (Fig. 4). Since then, advances in instrumental energy resolution and detector efficiencies
have been made to make neutron reactor sources extremely useful for a variety of research applications. Spallation neutron sources have produced the highest intensity fluxes of neutrons to date (Fig. 4). The increased flux has revolutionized the neutron sciences and, as this issue demonstrates, makes neutron analysis viable for a variety of studies of Earth materials, including under extreme conditions of pressure and temperature and even in the presence of a magnetic and/or electric field. The future is bright: currently under construction are the European Spallation Source (ESS) (Sweden) and the China Spallation Neutron Source (CSNS). These facilities, and upgrades to existing facilities, will help to meet the growing research demands of the scientific community and industry and to provide new neutron research capabilities not currently available.

**Neutron Methods and Opportunities**

When a neutron beam interacts with a sample, three possible phenomena can take place: (i) transmission, in which neutrons pass through the sample; (ii) absorption, whereby neutrons are taken in by the sample; (iii) scattering, in which the propagation direction of the neutron is deviated with respect to the original direction. Neutron imaging methods, such as neutron radiography and tomography, are based on the detection of the transmission of a neutron beam through an object. Neutron activation analysis (NAA) is a very sensitive method and is, therefore, used to analyze minor and trace elements in a sample. In particular, NAA has been used extensively for the determination of rare earth elements (REEs) in rocks and minerals because REEs have very high thermal neutron cross sections. Researchers are helped by having an online neutron activation analysis database which was developed by Bayrak et al. (2019). A particular advantage of NAA is that it does not destroy the sample, making it ideal to analyze works of art and historical artifacts (Glascocck 2014).

**Neutron Activation Analysis (NAA)**

Neutron activation analysis (NAA) is a mature and established method for determining the concentrations of elements in a material. This method relies on excitation by neutrons so that the treated sample emits gamma-rays that, in turn, allow the precise identification and quantification of elements in the sample. Neutron activation analysis is a very sensitive method and is, therefore, used to analyze minor and trace elements in a sample. In particular, NAA has been used extensively for the determination of rare earth elements (REEs) in rocks and minerals because REEs have very high thermal neutron cross sections. Researchers are helped by having an online neutron activation analysis database which was developed by Bayrak et al. (2019). A particular advantage of NAA is that it does not destroy the sample, making it ideal to analyze works of art and historical artifacts (Glascocck 2014).

**Neutron Imaging Methods**

The neutron imaging methods of neutron radiography and neutron tomography reveal the inner structure of an object. These techniques are based on the transmission and detection of a neutron beam passing through an object. When the beam passes through, the object’s different components attenuate the neutron beam differently, depending on their composition. This produces accurate 2-D and 3-D pictures of objects which provide information about the internal structure of an object (Winkler 2006). Large samples can be investigated with little or no radiation damage because of the high penetrating power of neutrons; light elements, such as hydrogen, can be detected in a sample dominated by heavy elements. Hess et al. (2011) describe how neutron computed tomography can be used as a tool for high-contrast imaging of natural glasses (including tektites), hydrothermally altered lavas, and tooth enamel microstructure. With its greatly improved spatial resolution, neutron computed tomography now promises to be a useful tool for a much wider spectrum of research in the Earth sciences. In addition, real-time imaging can also track the movement of material within objects, such as water in porous matrices. Applications of neutron imaging techniques in the Earth sciences are highlighted in the article by Artioli and Hussey (2021 this issue).

**Neutron Scattering Methods**

Neutron scattering experiments measure the number of neutrons scattered by a sample as a function of the wave vector change (Q) and the energy change (ΔE) of the neutron. The wave vector change is defined as $k_i - k_s$, where $k_i$ and $k_s$ are the wave vectors of the incident and scattered beams, respectively. The scattering process can be either elastic (no exchange of energy between neutrons and sample; $\Delta E = 0$), which is used for neutron diffraction, or inelastic (there is an exchange of energy with the sample; $\Delta E \neq 0$), which is used for neutron spectroscopy.

**Elastic Neutron Scattering (Neutron Diffraction)**

Neutron diffraction, or elastic neutron scattering, is used to determine the atomic and/or magnetic structure of a material. During elastic neutron scattering, there is no energy loss or from the atoms in the sample studied. The experiment consists of measuring the scattered intensity with varying scattering angles. The technique is similar to X-ray diffraction, due to the different scattering properties of neutrons versus X-rays, but yields complementary information. In particular, neutron diffraction is advantageous for the location of light atoms in a structure and for determining any magnetic ordering. Neutron diffraction is described in detail by Gatta et al. (2021 this issue).

The main types of neutron elastic scattering instruments are diffractometers (either for single-crystal, powder diffraction, or for diffuse scattering from amorphous materials), neutron reflectometers, and small-angle neutron scattering (SANS) instruments. Diffractometers probe the high Q
range (Q > 0.5 Å⁻¹) and are used to investigate the structures of crystalline systems. Reflectometers and small-angle neutron scattering instruments cover the low-Q range (Q < 0.5 Å⁻¹). The small-angle neutron scattering instrument is used to probe a material’s structure at the nanometer to micrometer scale and is described in more detail by Stack et al. (2021 this issue). Neutron reflectivity is a technique capable of determining the thickness and the chemical composition of one or several thin layers at a mineral surface. The typical order of magnitude of the thicknesses that can be measured experimentally lies in the range of 5 Å to 5,000 Å. The principle is to measure the coefficient of reflection (R) of a neutron beam sent in at a grazing incidence to the studied surface. Because it is a scattering technique, such a profile will be averaged on the whole surface and the technique and neutron reflectivity will not provide any information on the possible in-plane structure at the surface. Grazing incidence neutron scattering (GINS) is a special configuration of reflectometry used to characterize the “roughness” of surface structures with a length scale from nanometers to several microns. It is usually very valuable to combine neutron reflectivity with a second technique that enables in-plane structure information: this could be a scattering method, such as grazing incidence small-angle scattering (GISAS), or surface diffraction, or off-specular measurements, or a compatible microscopy technique (atomic force microscopy, Brewster microscopy). Example applications include the interrogation of the calcite–liquid interface (Stocker et al. 2012) and probing the substrate effects on biofilm formation on sapphire (Oleson et al. 2012). The general applications of neutron diffraction include

- The determination of crystallographic structures, especially those containing hydrogen (see Gatta et al. 2021 this issue);
- The determination of order/disorder in minerals as a function of pressure and/or temperature (e.g., Redfern et al. 1997);
- The determination of magnetic structures (Harrison 2006; Chakoumakos and Parise 2021 this issue);
- The determination of phase transformations and reaction pathways as a function of external parameters, such as pressure, temperature, and/or magnetic or electric fields (see Chakoumakos and Parise 2021 this issue);
- The analysis of texture and residual strain in rocks and minerals (e.g., Wenk 2006b);
- The investigation of noncrystalline structures, such as liquids or amorphous materials, by using diffuse scattering and pair distribution function analysis (see Benmore and Wilding 2021 this issue);
- The exploration of the internal micro-architecture of rocks (Radlinski 2006). Stack et al. (2021 this issue) describe how small-angle neutron scattering can be used to determine the pore structures of rocks and their change during gas, liquid, and solute imbibition and reaction.

**QUASI-ELASTIC NEUTRON SCATTERING AND INELASTIC NEUTRON SCATTERING**

Neutrons can lose or gain energy to or from the target atom during inelastic scattering, and this information can be used to describe how atoms move in a structure. Inelastic neutron scattering probes the atomic and molecular movements over a vast range of length scales, ranging from a few Ångstroms to tens of nanometers, and over timescales ranging from tens of picoseconds up to a few microseconds (Pic. 5). However, no single spectrometer can access this full range and, typically, three types are needed: a direct-geometry time-of-flight spectrometer (~10⁻¹¹ s), a backscattering spectrometer (~10⁻⁷ s), and a neutron spin echo spectrometer (~10⁻⁵ s). The time-of-flight technique is a general method for determining the kinetic energy of a traveling neutron by measuring the time it takes to fly between two fixed points whose distance is known. It is particularly useful in neutron spectroscopy where the energy of the scattered neutrons has to be determined (Copley and Udovic 1993). Inelastic neutron scattering is used to investigate vibrational properties of a material. Unlike infrared and Raman spectroscopy, there are no selection rules for inelastic neutron scattering. Therefore, the entire frequency distribution of the vibrations of the material (the vibrational density of states) can be determined and the thermodynamic properties of the material can be calculated (Ross 1992; Chaplot et al. 2002).

Quasi-elastic neutron scattering is a very low-energy inelastic process which usually manifests itself as a broadening of the elastic line that is most commonly the result of diffusional (translational or rotational) motion of atoms. This method is described in more detail by Stack et al. (2021 this issue).

A quick overview of the types of information provided by neutron spectroscopy (Loong 2006; Parker et al. 2011) includes

- Rotational, acoustic, and vibrational modes in minerals
- Phonon dispersion curves and spectra of minerals
- Vibrational density of states and thermodynamic properties of minerals as a function of pressure and temperature
- Phase transitions
- Diffusional and hopping motions of atoms
- Magnetic and quantum excitations
- Crystal- and electric-field effects.

Thus, neutron spectroscopy provides insights at an atomistic level about phenomena such as the phonon softening associated with structural phase transitions, phase diagrams, melting, reactions at mineral–water interfaces, catalysis, mechanisms of fast-ion diffusion, the origin of negative thermal expansion and low thermal conductivity, to name but a few. There is a symbiotic relationship between theoretical interpretations and the practical analysis of the often-complex neutron data which, in turn, can validate the models used to calculate the phonon, elastic, and thermodynamic properties of a material. The integration of neutron spectroscopy with theoretical methods has been extremely successful in providing important insights about mineral properties relevant to mineralogy, geochemistry, and petrology. These insights will continue to grow as the flux increases at neutron sources.
**FUTURE OUTLOOK**

For over half a century, neutron-based studies have been used to determine the composition, structural details, and the dynamics of atomic arrangements in materials from measurements of absorption and scattering. Compared to X-rays, the application of neutrons in the Earth sciences is relatively recent, and Earth science users are still in a minority in the neutron community. That said, neutron scattering should be viewed as an essential technology for advancing Earth materials research because it provides information that cannot be obtained from any other research method. This is because neutrons are magnetically sensitive, nondestructive, and sensitive to the light elements. Potential growth of the neutron community is being realized because neutrons provide a unique, nondestructive method to obtain information ranging from the Ångstrom-scale of atomic structures and related motions to the micron-scale of material strain, stress, and texture, as well as the meso-scale of porous matrices and defects in materials and functional components.

The information provided by neutrons can provide a robust understanding of basic geologic processes—crustal subduction, earthquakes, and volcanic eruptions—due to such processes depending on the physical, chemical, and rheological properties of the materials involved (i.e., crustal and mantle rocks, magmas, and fluids). These, in turn, depend on the structure and properties of the constituent minerals and the associated hydrous components, which can be determined using the neutron techniques described in this issue. We envision that important advances will be realized in crystallography (e.g., atomic positions of hydrogen in diverse Earth phases), order/disorder effects in silicate melts, distribution of oxidizes, mineral magnetic structures, mineral physics at deep Earth and planetary pressures and temperatures, and the interrogation of anisotropy and residual strain relevant to rock mechanics, structural geology, and tectonics. New applications will range from the structure determinations of large crystals, to powder refinements, and to short-range order determination in amorphous materials. The pore features of rock matrices—size, distribution, connectivity, and roughness (“fractality”)—can be quantified across over six-orders of magnitude in spatial scale. Additionally, mineral structure, dynamics, and reactivity of fluids hosted in porous materials, or on mineral surfaces, can yield atomic/molecular-level details amenable for direct comparison with advanced molecular-level simulations. Finally, as a detailed understanding of more complex Earth materials becomes increasingly important to our economy and national security, neutrons will become ever more essential to answering some of our most challenging science and technology questions.

**ACKNOWLEDGMENTS**

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How is hydrogen distributed among minerals and how is it bonded in their crystal structures? These are important questions, because the amount of hydrogen and the bonding configuration of hydrogen in crystalline materials governs many of that material’s properties: its thermal and compressional behavior, P–T phase stability, rheology, and electrical conductivity. A reliable reconstruction of the Earth’s interior, or the prediction of mineral transformations in complex industrial processes, must account for these parameters. Neutron diffraction can locate hydrogen sites in mineral structures, reveal any static or dynamic hydrogen disorder, help define the libration regime of hydrogen, and elucidate hydrogen-bonding configurations. Thus, that most elusive element for X-ray probes is perfectly detectable using neutrons.

KEYWORDS: neutron diffraction; neutron scattering; hydrous minerals; hydrogen bond; atomic disorder

INTRODUCTION

Hydrogen, formed in the early universe, is the most abundant element in the Solar System. It constitutes 70.6 wt% of the Solar System’s mass, being present in the giant gaseous planets and, of course, the Sun. On Earth, hydrogen exists as water vapor in the atmosphere, as water and ice in the ocean and, on land, as supercritical fluids in volcanoes, as H₂O molecules and hydroxyls in hydrous and nominally anhydrous minerals in the Earth’s crust and mantle, and as hydrogen “dissolved” in metallic iron in the core. Wu et al. (2018) proposed a model for the origin of Earth’s water, which included contributions from chondrites and from the solar nebula. These authors concluded that the Earth stores the majority of its hydrogen on the inside, with roughly two ocean equivalents of water in the mantle and four to five oceans in the core (Fig. 1). There is a continuous mass transfer of water between the geosphere, hydrosphere, atmosphere, and biosphere, which is promoted by a series of endogenic and exogenic phenomena, all of which govern the so-called “water cycle” or “hydrogen cycle”. Vitale Brovarone et al. (2020) and Demouchy and Bolfan-Casanova (2016) provide a description of these terrestrial water and hydrogen cycles.

Therefore, hydrogen has been one of the most investigated chemical elements over the last three centuries, especially after its recognition as an element in 1766 by Henry Cavendish. A series of experiments, coupled with atomistic simulations, have been performed over the last century to explore the stability of hydrogen over a broad range of pressures and temperatures (Goncharov 2020). Despite its chemical simplicity, solid H₂ occurs in different polymorphs in response to the different P–T conditions. However, the existence of “metallic hydrogen” under extreme conditions is still matter of debate.

Hydrogen occurs in a variety of bonding configurations, most of which are polar, that cover the whole range from purely ionic bonds (H⁺⋅⋅⋅anions) to covalent bonds (O–H, C–H, N–H) and coordinative bonds (metal–H). A comparative analysis of approximately 5,600 mineral species shows that 55%–56% of those are H-bearing minerals. In its ionic form, hydrogen can also possess a negative character and so form compounds with more electropositive metals in the form of “hydrides”. Bindi et al. (2019) discovered the first natural hydride, which was of vanadium (VH₂).

Figure 1. Water circulation into the Earth’s deep interior. Figure kindly provided by M. Nishi.
When hydrogen is bonded to a more electronegative element, it can participate in a noncovalent bond, for which the electronegative element has a lone pair, and so form a “hydrogen bond”. In the H-bonding scheme, a donor (Dn) atom is a covalently bonded atom to hydrogen, at the same time as there being an acceptor atom (Ac, a lone pair on an electron-rich acceptor atom). The hydrogen bond is directional, and its bonding energy depends on the nature of the donor and acceptor elements and the geometrical configuration: that is, the Dn–Ac distance and the Dn–H−−−Ac angle. Hydrogen bonds can range from being very weak (<17 kJ/mol) to very strong (170 kJ/mol) (Libowitzky and Rossman 1996). The strong hydrogen-bond network in water controls its unusual thermophysical properties, such as its unusually large specific heat, high melting point, and large surface tension.

In this article, we describe how neutrons provide a powerful probe to detect hydrogen in the crystal structure of minerals, to reveal its bonding configuration, and to uncover the dynamics of hydrogen in minerals. This information is critical because hydrogen plays a key role in many mineralogical, geochemical, and petrologic processes. Hydrous minerals, for example, not only provide information about the role of fluids in the Earth’s crust but also help transport water deep into Earth’s mantle and so form part of the cycle that helps regulate the sustained presence of surface water on Earth. In addition, hydrous minerals have many technological applications for use as ion-exchange materials, highly selective molecular sieves, catalysts, ion conductors, and hydrogen storage materials.

**COMPARISON OF X-RAY AND NEUTRON RADIATION**

**Bragg Scattering**

The goal of Bragg-scattering, or diffraction experiments in general, is to compare diffracted intensities with possible structure-derived model intensities and to identify the best-fitting one. For powder diffraction experiments, which contain Bragg intensities at the corresponding positions of related lattice planes, 1/2θ diagrams are experimentally measured. Because the samples consist of randomly distributed crystallites, the 3-D orientation information is lost. These data are affected by instrumental parameters of the diffractometer (e.g., energy resolution, angular resolution, and collimation) and by sample-specific features (e.g., crystallites, size, and texture). The Rietveld method covers all these experimental aspects and allows for a full-profile fit in each 2θ range. Single-crystal diffraction experiments preserve the angular relationship between different lattice planes, which can be especially beneficial for studies of anisotropic features, as described in the examples below.

The different ways that X-rays and neutrons interact with matter explains why detailed studies use both kinds of probes (see Ross and Cole 2021 this issue). Electromagnetic X-ray radiation interacts with the electrons, where the electronic scattering power of an atom (f_e; the X-ray form factor) is proportional to the atomic number (Z; its shell electrons). For this reason, heavy atoms with many electrons show a higher scattering power than light elements: this explains why hydrogen has a low scattering power, even compared with second period elements. Moreover, electrons occupy a finite volume, of the same order of magnitude as the wavelength (λ). For X-rays, atoms, including H, are not point-like scattering centers. This leads to a rapid lowering of f_e at higher scattering angles, especially for larger atoms.

In contrast, neutron radiation is based on the particle–wave duality of the neutron. Its mass is ideal for exciting oscillations of the nuclei in hard matter. Neutron radiation not only interacts with the nuclear cores but also with the magnetic moments of atoms. The neutron analogue to the X-ray form factor is the scattering length (b), the value of which depends on the specific isotope and can even vary between nuclei of the same isotope due to spin–spin interactions. If all the nuclei have the same scattering length, then they can scatter constructively—giving rise to Bragg-like diffraction—and have a coherent (coh) scattering length (bcoh) averaged over the different nuclei, i.e., bcoh = <b>. In the case of incoherent (“inc”) scattering, the scattering length (binc) is the root mean square deviation of scattering lengths, i.e., binc = <b²> − <b>²)½ (Squires 2012). For most elements, the coherent scattering length and corresponding cross section (σcoh) dominates. Hydrogen is an important exception, having bcoh = −3.739 fm and binc = 25.274 fm (1 fm = 10⁻¹⁵ m). The incoherent scattering will result in a large background that might obscure the coherent scattering, this latter being needed to determine the structure of the material. This problem can be addressed by deuteronating the sample, exchanging deuterium (²H) for the hydrogen (¹H), because deuterium has bcoh = 6.671 fm and binc = 4.04 fm.

Thus, X-rays and neutrons yield different, but complementary, information in diffraction experiments. X-rays reveal the electron density in a crystal and, thus, they can potentially reveal information on chemical bonding; neutrons uncover exact atomic positions. This is especially true for polar X–H bonds determined using X-ray diffraction, as the valence-only charge density of hydrogen is polarized toward the heavier atom, resulting in the systematic underestimation of X–H distances. In addition, neutrons provide advantages over X-rays in studies of other light elements, such as lithium and beryllium. There is also another important aspect: local effects can have an impact on the spatial distribution of the scattered neutrons. One of the most prominent is the Debye–Waller factor—also known as the temperature factor or atomic displacement parameter—which describes the damping effect on Bragg intensities caused by oscillations of the atoms around their time- and space-averaged positions in a crystal. It is common for light elements, such as hydrogen, to show anharmonic effects. Thus, their constant nuclear scattering lengths for neutrons are of great advantage. It allows measurements with high statistics up to high momentum transfer, where anharmonic effects on the scattered intensities are more pronounced. Another process that can affect the intensities is absorption. For X-rays, penetration depths are usually in the range of a few microns to less than 1 mm, which limits diffraction experiments to sample diameters of typically below 0.3 mm. Conversely, thermal neutrons show, for most elements, penetration depths of several centimeters, meaning that large and complex sample environments can be easily accessed (see Chakoumakos and Parise 2021 this issue). On the other hand, neutron diffraction typically requires larger samples than those used for X-ray diffraction, which can present a significant challenge.

**Beyond Bragg Scattering**

Hydrogen is commonly involved in the formation of complex static and dynamic disorder. The Bragg diffraction experiments discussed above produce a structural model based on the projection of the whole crystal into a single average unit cell, which is assumed to follow strict translational symmetry in real space. However, all the diffuse scattering that arises from static and dynamic disorder, order on a short length scale, complex correlated defect structures, or even amorphous atomic arrangements is neglected. Scattering terms due to these phenomena are often found as weak contributions to the background or as small intensity variations of the Bragg intensities. If
information from Bragg scattering is complemented by that emerging from disorder phenomena, then total scattering techniques arise, and these can probe the total electron density in real space. A full discussion of total scattering methods goes beyond the scope of this article, and the reader is referred to Keen (2001) and Egami and Billinge (2012) for more details.

**Inelastic/Quasi-Elastic Scattering**

Although this article focuses mainly on neutron diffraction, both inelastic neutron scattering and quasi-elastic neutron scattering offer additional, powerful tools by which to investigate hydrogen in minerals. Inelastic neutron scattering and quasi-elastic neutron scattering provide information about hydrogen bonding within minerals and mineral surfaces, as well as dynamical information of how hydrogen “moves” in a structure. For example, inelastic neutron scattering came into use to investigate interlayer H2O molecules, hydroxyl groups, and hydrogen bonding in a variety of phyllosilicates and clay minerals (e.g., Cygan et al. 2015). Wang et al. (2014) determined the vibrational density of states of strongly H-bonded interfacial water on surfaces of metal oxides using inelastic neutron scattering. Understanding the structure and properties of water at metal oxide–water interfaces is of special importance because they determine and control specific chemical processes, such as catalysis or mineral growth and dissolution. The inelastic neutron scattering method can also provide insights about the behavior of molecular H2O in confined environments, as described below.

The quasi-elastic neutron scattering method offers a way to gain insights into the diffusion of hydrogen within materials and its transport mechanisms, i.e., by measuring the rates of the rotational and translational diffusional motions of bulk H2O molecules. Stack et al. (2021) described how quasi-elastic neutron scattering is applied to explore the diffusional dynamics at mineral–H2O interfaces and to investigate the mobility of H2O confined in a great variety of both organic and inorganic H2O-containing materials. Furthermore, the method has also been applied to study water mobility and fluid movement through porous rocks, a process that influences such fields as contaminant remediation, CO2 storage, and oil recovery.

**HYDROGEN IN MINERAL STRUCTURES: BONDING CONFIGURATION, LIBRATION, AND DISORDER**

**Structurally Incorporated H2O in Minerals**

Neutron experiments have been extensively used to study hydrous minerals and have played a crucial role in improving our understanding of the chemical and physical properties of crystalline minerals (Gies 2009). In the Earth sciences, the adjective “hydrous” is commonly used for all the mineral species that contain either hydroxyl groups or H2O molecules. Below, we use case studies from two different mineral groups, with differently bonded H2O, to illustrate the different ways that molecules interact with natural crystalline materials. These include examples of heteropolyhedral microporous framework compounds with “confined” H2O and of cyclosilicates with “ultracalined” H2O.

**MICROPOROUS FRAMEWORKS WITH “CONFINED” H2O**

There are several microporous frameworks containing H2O. The most studied are the zeolites, which have H2O molecules confined in channels: these molecules are hydrogen-bonded to the oxygen atoms of the aluminosilicate framework and/or to each other. Zeolites have attracted interest mostly for their use as molecular sieves, but they have also been proposed as hydrogen storage materials, forming the basis for a new field of technologically important compounds: the zeolitic imidazolate frameworks. Many neutron diffraction experiments have been carried out on zeolites, revealing details of the hydrogen bonding and showing that the confined H2O molecules in these open-framework materials are usually weakly bonded (Gies 2009). In contrast, there have been far fewer studies of heteropolyhedral microporous frameworks in which the H2O molecules are strongly bonded. Among those, it is worth noting two dimorphs: epididymite, which is orthorhombic (space group Pnma), and eudidymite, which is monoclinic (space group C2/c) and having ideal formula Na2Be2Si6O15·H2O (H2O ~4 wt%).

Gatta et al. (2008) performed a reinvestigation of the structure of these two dimorphs by single-crystal neutron diffraction at 298 K. The structure of these minerals is built on topologically different frameworks made by SiO4 and BeO4 tetrahedra. Sodium atoms are located in small cavities (~4–5 Å) and bonded to oxygen atoms of the tetrahedral framework and H2O molecules. The structure refinements allowed Gatta and colleagues to unambiguously locate all the H sites. The configuration of the H2O molecules and hydrogen bonds in epididymite and eudidymite are shown in Figure 2. In epididymite, two strong hydrogen bonds
occur with the framework oxygen atoms. The unique H₂O molecule appears to be significantly bent, having an H–O⁻Dn–H angle of ~102°, compared to ~106° in the (ideal) water molecule. This value is unusually low, although still in the range of the H–O⁻Dn–H angles in solid-state materials.

The configuration of the H₂O molecules and hydrogen bonding in eudidymite is even more complex. As shown in Figure 2, two symmetry-related and mutually exclusive O⁻Dn sites occur (with site occupancy 50%) at only 0.37 Å apart, giving two statistically distributed configurations of the H₂O molecule in the eudidymite structure. The H₁–O⁻Dn–H₂ angle is ~104°, slightly less compressed than in epididymite. The (static) position disorder of H₂O in eudidymite can be ascribed to the fact that the molecules were at the center of the channel, then the H···O distances would be too long and the H–O⁻Dn–H angle would be far from an energetically favorable configuration. The strong hydrogen bonding in these dimorphs and the arrangement of H₂O molecules in the small channels of epididymite and eudidymite control their physical and chemical properties. For example, the temperature of dehydration is unusually high (T > 800 °C), and the heat capacities and entropies are generally higher than those found for zeolites (Geiger et al. 2010).

CYCLOSILICATES WITH “ULTRACONFINED” H₂O

Molecular H₂O is a common constituent of cyclosilicates that have 1-D channels. This is the case of beryl and cordierite. Beryl is a nominally anhydrous mineral that has the ideal formula Al₂Be₃Si₆O₁₈. However, alkali cations (Cs⁺, Rb⁺, K⁺, Na⁺) and H₂O molecules can occur within the six-membered ring channels along [001]. Many single-crystal X-ray diffraction and vibrational spectroscopy experiments have shown how H₂O, along with alkali cations, are located in the ~4.9 Å diameter channels running parallel to [001] (see Gatta et al. 2006 and references therein). Because the confinement of H₂O is largely 1-D and the diameter of the confining channel (~5 Å) is not much bigger than that of the confined molecule (diameter of H₂O is ~2.75 Å), the H₂O in beryl is usually referred to as being “ultracarved”.

Two single-crystal neutron diffraction experiments performed by Artioli et al. (1993) and Gatta et al. (2006) revealed two different H₂O configurations that appear to be controlled by the weight fraction of H₂O and alkali cations (i.e., the channel content). First, the H₂O/alkali-rich beryls (i.e., H₂O + Na₂O + Cs₂O > 3 wt%) show a configuration of the H₂O with the oxygen site on the 6-fold axis and hydrogens distributed around the 6-fold axis with the H+H vector lying on a plane parallel to [001] (type-II H₂O) (Fig. 3). Second, for the H₂O/alkali-poor beryls (H₂O + Na₂O + Cs₂O < 1.5 wt%) the O site lies on the 6-fold axis and the H sites are distributed in six equivalent positions around the H₂O, two symmetry-related H+H vectors oriented almost parallel to [001] (i.e., at ~4° from [001]) (type-I H₂O) (Fig. 3). No evidence of interaction could be inferred via hydrogen bonding between H₂O molecules and framework oxygens in either beryl configuration. In the presence of H₂O, there is only a weak interaction with alkali cations lying along the channels.

Additional experiments based on inelastic neutron scattering, quasi-elastic neutron scattering, dielectric spectroscopy, and density functional theory ab initio simulations, were later performed on beryl and revealed a new state of H₂O within the mineral (Anovitz et al. 2013; Kolesnikov et al. 2016). There is a novel “quantum tunneling state” of the H₂O molecule that is confined in the ~4.9 Å channels of beryl. In this state, the oxygen and hydrogen atoms of the water molecule are “delocalized” and are, therefore, simultaneously present in all six symmetrically equivalent positions in the channel at the same time, an effect that can only occur in quantum mechanics.

Hydroxyl (OH⁻) in Minerals

The majority of the so-called “hydrous minerals” contain hydroxyl (OH⁻) groups rather than H₂O molecules. Here, we focus on one of the most common groups of minerals of the Earth’s crust: the phyllosilicates. These minerals reveal differing bond configurations that control, in part, their physical properties.

PHYLLOSILICATES

Among phyllosilicates, talc and muscovite represent two examples in which the hydrogen-bond configuration is rather unusual. Talc occurs as a natural product of metamorphism or of the hydrothermal alteration of Mg-rich ultramafic rocks, and its ideal chemical formula is Mg₃Si₄O₁₀(OH)₂. Talc is also one of the most important industrial minerals, because of its low coefficient of friction, chemical inertness, and hydrophobicity. It contains ~5 wt% H₂O. The crystal structure of talc consists of a sheet of linked [Mg₄O₉(OH)₂] octahedra (“O³”), sandwiched between two sheets of SiO₄ tetrahedra (“T⁴”) combined to six-member rings, giving the so-called “T–O–T” layered structure (Fig. 4). The T–O–T layers are charge neutral, held together by weak van der Waals attractive forces, resulting in the extreme softness of this mineral. The crystal structure of the Tᶜ-talc (space group C̅T) was re-investigated by single-crystal neutron diffraction at 20 K (Gatta et al. 2013) and within the framework of a multimethodological study in which the thermal and compressional behavior were also investigated. Neutron structure refinement revealed an unusual hydrogen-bonding scheme in talc, shown in Figure 4, with one donor site and three acceptors, i.e., a trifurcated configuration. The three acceptors belong to the six-member ring of tetrahedra juxtaposed to the octahedral sheet (Fig. 4). The O⁻Dn–H vector is perpendicular to the octahedral sheet. The vibrational regime of the proton site appears to be only slightly anisotropic. With such a configuration (i.e., long O⁻Dn···OAc distances, low O⁻Dn–H···OAc angular values), the hydrogen bonds are very weak in energy.

Figure 3 (A) Photo of the mineral beryl. (B) Schematic configuration of the H₂O orientation in beryl. In H₂O/alkali-rich beryl, oxygen atoms lie on the 6-fold axis, hydrogen atoms and H–H vectors lie on [001] (type-II H₂O). (C) In H₂O/alkali-poor beryl, oxygen atoms lie on the 6-fold axis, H–H vectors are oriented almost parallel to [001] (type-I H₂O). Colors: O sites in red; H sites in yellow.
The structure of muscovite, which has the ideal composition KAl_2(Si_3Al)O_10(OH,F)_2, is more complex. Muscovite is a dioctahedral mica with “T–O–T” layers connected by interlayer cations (mainly K). The presence of Al as the principal octahedral cation generates an octahedral layer in which 2/3 of the three potential octahedral sites are populated (Fig. 4). This, in turn, leads to a different H location and hydrogen-bonding configuration compared to talc. A series of studies based on neutron diffraction methods were devoted to muscovite (see Gatta et al. 2011 and references therein). Gatta et al. (2011), using single-crystal neutron diffraction analysis, collected diffraction data at 295 K and 20 K on a 2Mf-muscovite and provided high-quality structure refinements with all the atomic sites (including H) modelled anisotropically. In addition to showing that a trifurcated hydrogen-bonding scheme occurs, in which the three interactions are very weak, the refinements proved that only one independent H site occurs in the structure of muscovite, with no evidence of static or dynamic disorder, which was previously a matter of controversy. The neutron refinements also revealed details not easily determined by X-ray diffraction. They showed, for example, that the atomic displacement ellipsoid of hydrogen has a pronounced anisotropy, and that a disordered Si/Al distribution occurs on the two independent tetrahedral sites.

The details of the hydrogen environment in muscovite and talc were only revealed by neutron diffraction. The results were important in understanding the physico-chemical and elastic properties of the minerals. Specifically, different orientations of the O–H vector in phyllosilicates can play an important role in their compressional and thermal expansion behavior, which are notably anisotropic.

**NOMINALLY ANHYDROUS MINERALS**

Other rock-forming minerals, which usually occur in their anhydrous form, can incorporate hydrogen at a significant level. Neutron diffraction experiments reveal how hydrogen is incorporated in such minerals, thereby determining their hydrogen storage capacity. This is especially important in studies of the Earth’s interior, because even trace amounts of hydrogen in a mineral structure can affect the propagation of seismic wave velocities and rheological properties of mantle minerals (e.g., Karato 2006).

Silicate garnets are important constituents of the Earth’s crust and mantle. Hydroxyl can be incorporated in garnets and other materials via the so-called “hydrogarnet substitution”, in which SiO_4^{2−} is replaced by four OH^−. Lager et al. (1987) performed seminal time-of-flight powder neutron diffraction experiments on the hydrogarnet katoite, Ca_3Al_2(O_4H_4)_3, at 300 K, 200 K, and 100 K. Rietveld structure refinements on the deuterated sample elucidated the positions and anisotropic displacement tensor of the (unique) H site (Fig. 5). Lager and colleagues found that the displacement ellipsoid (which represents magnitudes and directions of vibration of an atom, due to the always-present atomic motion) has a pronounced anisotropy, even at 100 K. Weak hydrogen bonds, having a bifurcated configuration, occur with oxygen vertices of the tetrahedron and act as donors and acceptors. Recently, Kyono et al. (2019) investigated the stability of katoite in situ at high pressures and temperatures using neutron diffraction. They discovered that katoite remains hydrated up to 850 °C and 8 GPa, suggesting that this mechanism might transport “water” into the Earth’s mantle.

Two high-pressure polymorphs of olivine are wadsleyite and ringwoodite. Both polymorphs are major minerals of the Earth’s transition zone and may also serve as a large internal reservoir for hydrogen. Recently, a natural transition-zone ringwoodite, containing at least 1.4 wt% of H_2O, was discovered as an inclusion in diamond (Pearson et al. 2014). Subsequently, single-crystal neutron diffraction experiments elucidated the storage capacity of hydrogen in wadsleyite and ringwoodite (Purevjav et al. 2016, 2018): these experiments determined how the hydrogen exchange mechanisms are quite different in the two polymorphs. In
wadsleyite, there is only one oxygen site (out of four) that is available to be exchanged by OH− (Purevjav et al. 2016). In ringwoodite, however, a hydrogen can exchange not only with the Mg or Fe in the octahedra but also with the Si in the tetrahedra (by substitutions as 1Mg2+ + 1Si4+ ↔ 2H+), 2Mg2+ + 1Si4+ ↔ 6H+, or 4Mg2+ + 1Si4+ ↔ 12H+, requiring vacant Mg and Si sites (Purevjav et al. 2018). Therefore, ringwoodite has a larger “water” capacity in the lowervalent region of the transition zone compared to that of wadsleyite in the upper half of the transition zone. The difference is a vital clue towards understanding why these dense mantle minerals show distinctly different softening behaviors after hydration.

CONCLUDING REMARKS

In this article, we have shown the benefits of using neutron scattering techniques, especially diffraction, for the location of the hydrogen sites in a mineral (even with concentration of a few thousands ppmw), the description of the static or dynamic disorder of hydrogen sites, the liberation of hydrogen through a full description of the displacement tensor from the center of gravity, and the hydrogen-bonding configuration in minerals. This, in turn, provides the essential information needed to model the physical and chemical properties of the hydrogen-bearing minerals in either natural or industrial contexts. A mineral’s thermal or compressional behavior, its P–T phase stability, and its leaching or catalytic activity are all influenced by the hydrogen-bonding scheme. Past limitations in the experimental need to use large crystal volumes or masses of polycrystalline samples, have been largely overcome by more powerful or more diverse neutron sources and instruments.

We hope that this article will further stimulate the mineralogical community’s interest in developing and making greater use of the range of currently available neutron-based techniques.

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**Nanoscale Structure and Dynamics in Geochemical Systems**

Andrew G. Stack¹, Hsiu-Wen Wang¹, and David R. Cole²

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### INTRODUCTION

The structure and dynamics of water, aqueous species, and the interaction of these substances with Earth materials, all play essential roles in geochemical processes. Understanding the interaction between a solute and its solvent is critical for predicting solid solubilities, the kinetics of mineral and amorphous phase growth and dissolution, the weathering or alteration of geological materials, and many other properties or processes. Neutron scattering methods described by Ross and Cole (2021 this issue) provide the opportunity to quantify these processes.

We begin by showing how the nature and extent of ion pairing and chemical complex formation can be revealed in aqueous solutions. Next, we offer examples of how mineral surface reactivity is interrogated, demonstrating how the nanoscale structure of the mineral–water interface modifies reactivity compared to bulk phases. Finally, we show how neutron scattering provides a unique window on fluid structure and dynamics within nanoporous media, where the reactivity of the mineral–water interface is intrinsically coupled to the rate of transport. The information obtained from neutron scattering is dramatically enhanced by a rigorous comparison to atomic-level simulations, allowing an unambiguous interpretation of atomic structure and validation of the molecular model. This can then be used to predict other geochemical processes with a greater degree of confidence.

This article focusses on three methods: neutron diffraction, quasi-elastic neutron scattering, and small-angle neutron scattering. Neutron diffraction permits the direct determination of pair distribution functions of solutions and materials, which provides molecular-level structural information about the distribution of distances between atoms in the sample. Neutron diffraction with isotopic substitution (NDIS), a technique unique to neutron scattering, yields increased chemical specificity of the signal by eliminating contributions from certain elements by substituting a different isotope of one element in the sample, changing its scattering. Quasi-elastic neutron scattering (QENS) yields diffusional motions of hydrogen-bearing solvent molecules (such as water) on the picosecond-to-nanosecond timescale. Applying a validated computational model allows for the extraction of surface site-specific solvent exchange rates, a key parameter for understanding mineral reactivity (Casey 2015). Small-angle neutron scattering is a method analogous to diffraction, but the scattering is from phase boundaries instead of atoms, and yields the characteristics of pore structures from the nanometer-to-micrometer scales: larger scales can be achieved by combining with the related technique of ultra-small neutron scattering. Performing small-angle neutron scattering in situ permits quantification of poorly constrained rates of crystal growth. The dynamical behavior of fluids and gases contained within porous solids can also be observed using QENS. The richness and complexity of fluid behavior (e.g., phase transitions, molecular orientation and relaxation, diffusion, adsorption, wetting, capillary condensation) in confined geometries continues to be the focus of numerous applications of neutron scattering.

**COMPLEX ION ASSOCIATION IN AQUEOUS SALT SOLUTIONS**

The study of aqueous solution structures by total scattering (diffraction) methods has been well-established since the early 1900s. Modern high-flux neutron sources, combined with rigorous comparison to atomic-scale simulations, are beginning to reveal the rich structural and chemical complexity of these systems that has hitherto been understood only in the most general terms. It is long-known that contact and solvent-separated ion pairs, or monomeric and dimeric ion complexes, may exist in a given solution. One can find a multitude of measurements of the extent and nature of ion-pair and complex formation in the literature. Although numerous quantitative estimates of the thermodynamics of ion association exist, they are often derived from macroscopic solution properties (e.g., conductivity...
measurements). This approach is simple and more-or-less robust, but it is not an actual measurement of the extent of ion-pair formation. It does not include the molecular-scale information necessary to predict reaction mechanisms, nor does it allow us to move beyond classical concepts of the nonideality of solutions. More recent evidence argues for higher-order extended networks of ions (Gebauer et al. 2018); however, quantitative estimates of the thermodynamics of their formation are difficult to make.

This situation may be rectified by neutron total-scattering data, used to derive the pair distribution function (PDF) (Ross and Cole 2021 this issue). A PDF shows atomic-level structure in terms of a series of peaks (and valleys), with positions determined by the distances between atoms and with intensities controlled by the concentration of each element and their propensity to scatter neutrons (or X-rays). Integration of the PDF peaks yields coordination numbers. Whereas X-ray PDF analysis tends to exhibit a much stronger signal than neutron PDF, X-ray PDF is weighted towards heavier elements and is typically used for distances <1 nm for solutions. Neutron total scattering/ PDF techniques, on the other hand, are uniquely capable of capturing the extent of ion association due to their sensitivity to both light elements (H and O) and heavier elements (solute cations, anions) with the added ability to observe longer-range structures (e.g., several nanometers using the Nanoscale Ordered Materials Diffractometer instrument, part of the Spallation Neutron Source at Oak Ridge National Laboratory in Tennessee, USA). Because the neutron scattering contrast between elements varies with the isotope, one can further utilize isotopic substitution (e.g., D for H) to manipulate scattering from a sample.

In NDIS, isotopic substitution is taken to the extreme by observing two solutions that are identical, except in the composition of the isotope of one the elements (e.g., 35Cl vs. 37Cl). The difference in scattering between the two solutions is then taken, which yields the PDF with respect to just the labeled element (as opposed to all the atoms in the sample). This procedure removes the vast majority of peaks in the PDF (e.g., those from bulk water), immensely simplifying the interpretation. However, it also has the potential to introduce error because any contaminant present in one sample and not in the other will show up as a peak (or valley). Similarly, concentration differences will also cause peak intensity to vary, interfering with the calculation of the coordination number during integration of the PDF. And because protium (i.e., 1H) is highly effective at scattering neutrons in contrast to OD (Ross and Cole 2021 this issue), any additional hydrogen, such as from ambient water vapor in the air, will increase the background noise. Thus, extreme care is needed in the preparation of samples for making robust NDIS measurements.

As an example of this method, Wang et al. (2018) conducted a benchmark study of oxyanion solution structure for saturated potassium nitrate solution (3.4 mol KNO3/kg D2O), using nitrogen and oxygen isotopes on the nitrate-N or nitrate-O sites (Fig. 1 TOP LEFT). Historically, NDIS measurements with oxygen isotopes (16O vs. 18O) were not thought to be possible because the difference in scattering would be too small. Recent work has shown that it is possible, just not easy (Fischer et al. 2012). The total scattering data from both the nitrogen-label and the oxygen-label is shown in Figure 1 BOTTOM LEFT, as are the PDFs with respect to these elements (Fig. 1 BOTTOM RIGHT). The attraction of doing such a difficult experiment is that, by focusing on the coordination oxygen on the oxyanion rather than its central atom, one can obtain a much less ambiguous coordination number, because one is measuring nearest neighbors and not next-nearest neighbors. Wang et al. (2018) revealed a coordination number of 1.3 ± 0.4 D(H)-bonded water molecules per oxygen on the anion (3.9 ± 1.2 for the whole nitrate), a smaller number than typically observed, but also a much higher precision measurement than was previously possible. The low water coordination number suggests that contact ion pairing in that solution is significant: classical molecular dynamics simulations calibrated to the NDIS data gave ~1–2 K+ per NO3− oxyanion (Fig. 1 TOP RIGHT). The extent of ion association in KNO3 solution, which is at saturation (3.4 mol KNO3/kg D2O), was found to be limited to simple contact ion pairs. No evidence for complex ion networks, clusters of solute species, or even solvent-separated ion pairs was found in this particular system. However, clustering of solute species has been observed using total scattering in more highly concentrated solutions than those found in typical geochemical systems (e.g., ~18 mol NaOH/kg D2O) (Semrouni et al. 2018). While there is still work to do to improve the computational models, a rigorous comparison to PDF data is opening a new path to molec-

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**Figure 1** Determination of an atomic-scale solution structure using neutrons. (top) Schematic of an experiment using neutron diffraction with isotopic substitution (NDIS). The difference in scattering of two solutions, which only vary in the isotope of one element, is taken, yielding the structure of the solution surrounding that element. Symbols: H = hydrogen; D = deuterium; T = tritium; nat = natural; O=Oxygen on a nitrate molecule; m = mol KNO3/kg D2O; inter. = intermolecular PDF (excluding structure from within the nitrate molecule); intra. = intramolecular PDF (including structure from within the nitrate molecule); ΔF norm = normalized structure factor that shows the difference in scattering as a function of wave vector (q); ΔG norm = PDF, showing probability of finding atoms at distance r from each other in the sample. (bottom left) Data from an NDIS experiment on a 3.4 mol KNO3/kg D2O solution using the two different labels of 15N and 18O. (bottom right) Normalization and a Fourier transform of the pair distribution function. Because the contribution to the PDF from the nitrate molecule is known, it can be subtracted out (intramolecular only), yielding the solvation structure. Adapted with permission from Wang et al. (2018). Copyright (2018) American Chemical Society.
ular-based arguments for macroscopic thermodynamic properties, such as activity coefficients and an improved understanding of the relationship between concentration and activity.

Moving beyond average structures of complex aqueous solutions, QENS probes the diffusional motions of hydrogen-bearing species that have characteristic times from ~1 ps (e.g., self-diffusion of bulk water at room temperature) (Teixeira et al. 1985) up to several nanoseconds (diffusion of viscous solutions and some solvent exchange reaction rates on ions and surfaces). Diffusional characteristics are quantified either by fitting the data to an empirical model or by comparing the data to the predictions of computational simulations. To put this dynamic range into perspective, QENS measures slower motions than bond vibrations, but faster than those observable by nuclear magnetic resonance methods. Both QENS and nuclear magnetic resonance are also sensitive to different types of motions: QENS can differentiate between the rotational and translational motions of protons (often on water molecules), depending on how the signal changes as a function of the scattering angle, whereas nuclear magnetic resonance is sensitive to the motions of a specific isotope (e.g., $^{17}$O).

The dynamics of aqueous solution components observed by QENS are connected to their reactivity. For example, Wang et al. (2019) were able to use QENS to relate ion–water diffusible mobilities and dynamic properties of water to induction times for nucleation and phase selection in highly concentrated aluminate solutions containing sodium (Na$^+$) or potassium (K$^+$) as counter ions. In the presence of sodium, the diffusional motions of water were up to an order of magnitude smaller than those within the potassium-containing solution. Additionally, more local or confined motions were observed in sodium-containing solutions, which was interpreted as sodium promoting locally ordered structure of the aluminate and solvent species that, in turn, frustrates diffusion. In potassium-containing solutions, less confined motions and faster diffusion were observed. These microscopic dynamics correlate with the induction times for aluminum (oxy)hydroxide crystallization and mechanisms, where potassium-bearing solutions crystallized within a few hours to a day, but the equivalent sodium-bearing solution did not crystallize at all, instead forming a gel after 3–6 months. Although the specifics of how a counterion might control nucleation mechanisms are not known, it is clear that solvent exchange dynamics play a role (e.g., Casey 2015). More generally, this conclusion is also true for other geochemical processes, such as mineral dissolution (Casey 2015). By quantifying the rates of solvent exchange in aqueous solution using QENS, coupled to the improving of our understanding of the structure of aqueous solutions measured by total scattering/PDF, it is hoped that these techniques will allow us to discover the specific reaction mechanisms for geochemical processes. In turn, these discoveries will allow us to develop robust quantitative predictive models for the rates of geochemical processes occurring under a variety of circumstances: weathering, carbon sequestration, mineral replacement reactions, leaching, contaminant remediation, and so on.

**REACTIVITY AND SOLVENT EXCHANGE AT MINERAL–FLUID INTERFACES**

When bulk fluids come in contact with a mineral surface, a nanoscale interfacial region is created with structural and dynamic properties that may affect, or even control, diffusive transport and reactivity of the dissolved species and the solvent molecules within it. Surface sites of a mineral have a limited capacity to adsorb within the interlayers of montmorillonite clays, leading to expansion of the distance between clay particles. This piece of information is critical to understanding how CO$_2$ moves in the subsurface and suggests that there is a tendency for self-sealing of caprocks above a reservoir which, in turn, could enhance the storage security of CO$_2$.

As above, dynamical information for interfacial water and solvents is a key piece of information that can be obtained by neutron scattering. For interfacial solvents, one typically employs either QENS or inelastic neutron scattering. As above, QENS tends to help determine dynamical motions of species in the picosecond-to-nanosecond timescale, such as diffusional and solvent exchange motions at the interface, whereas inelastic neutron scattering is sensitive to faster, vibrational motions of various bond types. Commonly with QENS one might probe the timescale of diffusive motions of water adsorbed to a nanoparticulate mineral that has a high surface area. By necessity, only a few monolayers of adsorbed water are possible to measure, such as those that form when a mineral is exposed to humid air. Otherwise, the spectra will be dominated by the contribution from the bulk fluid. By comparing the timescales of these motions to those of self-diffusion of water, one can determine the
extent to which the kinetics of diffusion are slowed at the interface (Teixera et al. 1985). Comparison to molecular models allows one to interrogate different types of water at the interface, depending on their bonding environments (Mamontov et al. 2008). However, some surprising behavior has been observed in low-water environments, such as very dry surfaces or the molecular-level channels within some hydrated minerals. This includes quantum tunneling of hydrogen atoms during rotational motions of water in beryl (Kolesnikov et al. 2016) and a loss in the ability to freeze (Mamontov et al. 2009).

One challenge with this method is that the large number of different surface sites will have varying solvent exchange rates (Fig. 2). Such a large array of motions with different timescales creates the danger that the empirical fits to, say, a jump diffusion model respond more to the dynamic range of the spectrometer rather than anything intrinsic about the system. In Stack et al. (2016), this issue was partially addressed by running a series of classical molecular dynamics simulations of the interface (Fig. 2B). The water trajectories of the simulations were Fourier transformed and convoluted with the measurement of the background scattering from the experiment (i.e., the resolution function) (Fig. 2A). This allowed Stack and colleagues to make a direct comparison of what the model predicted the QENS data should look like. From there, the researchers interrogated the model for the solvent exchange rates of as many surface sites as possible (Fig. 2C). An outstanding issue, however, is that only the interface from a single crystallographic surface was considered in that study. Dealing with complex particle morphologies is an as-yet unsolved problem.

**FLUIDS IN NANOPORES MEDIA**

Geological fluids containing inorganic and organic solutes (including hydrocarbons) and gaseous species (e.g., CO₂, CH₄) can occupy nanopores, grain boundaries, and fractures in complex heterogeneous Earth materials. The collective structure and properties of bulk fluids are altered by solid substrates, with the effects of confinement between two mineral surfaces, or in narrow pores, dependent on the interplay of the intrinsic length scale of the fluid and the length scale of confinement (Cole and Striolo 2019). The combined effect of intermolecular forces and fluid confinement results in unique (but poorly constrained) perturbations to a wide range of thermodynamic, thermophysical, and transport parameters, different from those observed in the bulk phase (Gubbins et al. 2014). Because the interfacial areas (fluid–fluid and mineral–fluid) in Earth materials may be relatively large, confinement effects may control transport behavior and chemical reactivity. However, direct observations and modeling of the physical (transport) and chemical (reactivity) properties are challenging when considering the smaller length scales typical of pore and fracture features and their extended three-dimensional network structures.

In this context, neutron scattering, in concert with molecular-level (or larger) simulations, plays a vital role in examining the behavior of fluid–solid interactions in nanopores. The properties of neutrons make them an ideal probe for comparing the properties of bulk fluids with those of fluids in confined geometries. Thus far, neutron scattering measurements of Earth materials containing fluid-filled pores has centered primarily on clays and other layered silicates (e.g., serpentine), zeolites, coal, and certain rock types such as shale, limestone, and sandstone. As one might expect, much more neutron scattering research has been performed on engineered materials, such as micro- and mesoporous silica and carbon with relevance to controlling adsorption, chemical separation, nanofluidics, catalysis, batteries, and supercapacitors (Gautam et al. 2017). However, in many cases these systems can be used as proxies for structural and dynamical behavior of natural fluids in Earth materials.

The unique structural properties of confined liquids can be assessed using coherent scattering techniques: neutron diffraction, and small-angle neutron scattering. There has been considerable attention focused on determining the structure of water confined in hydrophilic systems, such as mesoporous silica and clays, using neutron diffraction complemented by a classical molecular dynamics simulation, which is an approximate simulation method commonly used to probe structure, dynamics, and energies at the atomic scale. Neutron diffraction studies indicate that confined water molecules form hydrogen bonds to each other and to the silicate surface such that their local environment relaxes to being close to that of a bulk water structure beyond roughly two molecular layers of the surface (Findenegg et al. 2008).

**Figure 2** Solvent exchange from quasi-elastic neutron scattering (QENS) experiments. (A) A barite (BaSO₄) nanoparticle powder with only a few monolayers of water adsorbed is measured using QENS at six different temperatures (K). Data is intensity of scattering as a function of energy transfer. Larger values of energy transferred often indicate faster motions. Solid lines are the classical molecular dynamics fit; points are the experimental data. (B) A computational molecular dynamics model is run at the same adsorbed water concentration as in the experiment and is fit to the data in Figure 2A. Water is color-coded by the type of surface site it is bound to: purple = barium; brown = sulfate; white = water bound to other interfacial water. “High” refers to barium surface site in a high position relative to the interface; “low” refers to barium surface site in a low position relative to the interface; “residence time” is the average time a water molecule is bound to a specific surface site. (C) Once validated, the solvent exchange rates for the four types of surface site are interrogated (high and low; barium and sulfate sites). REPRODUCED FROM STACK ET AL. (2016) WITH PERMISSION FROM THE PHYSICAL CHEMISTRY CHEMICAL PHYSICS OWNER SOCIETIES.
Neutron diffraction has allowed an exploration of the structure of the double layer that forms in swelling clays (e.g., vermiculite and smectite) and how interlayer cations are controlled largely by cation size and charge, in a manner similar to that observed for ions in concentrated aqueous solutions. Studies have revealed no significant water motion in the anisotropic, as in clays such as vermiculite, where QENS (e.g., vermiculite and smectite) and how interlayer cations can progress from nonsolvated inner-sphere complexes to solvated outer-sphere complexes. Neutron diffraction and complementary classical molecular dynamics simulations indicate that the coordination of the interlayer cations with water and clay surface oxygens is controlled largely by cation size and charge, in a manner similar to that observed for ions in concentrated aqueous solutions.

There is a tendency for the clay mineral structure to exert leading to nonsolvated inner-sphere complexes. Conversely, smaller monovalent and divalent cations, such as Li⁺, Ca²⁺, and Ni²⁺, tend to form highly solvated outer-sphere complexes.

Our ability to extract hydrocarbon gases (methane, ethane, propane) and oil from shales has significantly altered the global energy landscape and has led to economic growth and environmental impacts due to water use and subsequent disposal. Recent developments involving the recovery of methane, ethane, and propane from gas shales have sparked great interest in the geo-neutron science community to explore the behavior of these fluids, as well as CO₂ in nanoporous regimes (Ruppert et al. 2013; Xu 2020). Interest in the behavior of supercritical CO₂ in nanoporous regimes has also increased due to supercritical CO₂ being used to enhance hydrocarbon recovery. There is also the need to understand the behavior of supercritical CO₂ as part of subsurface storage projects to mitigate atmospheric emissions.

Rother et al. (2014) combined small-angle neutron scattering (SANS), gravimetric adsorption, and molecular simulations to probe sorption of supercritical CO₂ as a function of temperature and pressure using nanoporous silica as a model substance (Fig. 3). The sorption phase is significantly denser than the bulk fluid at low density (low pressures), but of equal or lower density than the bulk fluid at high pressures. At the sorption maximum, which corresponds approximately with the bulk critical density, the sorption phase is up to ~3 times denser than the corresponding bulk fluid. The silica pore walls with mesh-like nanometer structure provide a random network of adsorption sites, acting as anchor points for a continuous sorption phase. This pattern of fluid enrichment and then depletion has been measured for other weakly wetting fluids like methane, ethane, and propane.

The dynamical behavior of water and other geo-fluids in subsurface porous matrices impacts a variety of geochemical phenomena, including ion adsorption and exchange, mobility of contaminants, weathering, hydrothermal alteration, and fluid flow, to name but a few. The type of diffusive motion exhibited by hydrogenous fluids most affected by nanoconfinement includes both translation and rotation typically probed by QENS (picoseconds to nanoseconds) and neutron spin echo (nuclear magnetic resonance spectroscopy which probes motions on the timescale of tens of nanoseconds). Fundamentally, as the pore size decreases so does the mobility of water, as demonstrated, for example, by Osti et al. (2016) who used QENS to constrain the translational diffusivity of water in mesoporous silica (4–8 nm) with varying levels of surface hydration. This motion can be isotropic, as is commonly the case in cylindrical-pore materials such as silica. Conversely, water diffusion can be anisotropic as in clays such as vermiculite. Recent studies have revealed no significant water motion in the direction perpendicular to the clay platelets. This implies a 2-D motion of water along the planes of the platelets. The diffusion of this confined water tends to be slightly reduced compared to the bulk. Furthermore, order-of-magnitude decreases in water mobility compared to bulk water can occur in nanopores containing aqueous solutions comprised of structure-making ions (XCl₂ with X = Ba²⁺, Ca²⁺, Mg²⁺) (Baum et al. 2019).

The fact that hydrogen has a much larger neutron scattering cross section compared to deuterium also provides the opportunity to interrogate the behavior of one hydrogenous fluid in the presence of another that is deuterated. Gautam et al. (2019) used QENS to probe the interaction and dynamics of propane (C₃H₈) mixed with “invisible” D₂O.
in 4 nm silica pores and so demonstrated the two types of probe behavior: a slow diffusion component with longer residence times and jump lengths associated with fluid close to the pore wall, and a faster component with shorter residence times and shorter jump lengths located in the center of the pore.

OUTLOOK

The advances that neutron scattering are providing rely on its sensitivity to light elements, especially hydrogen, and that scattering intensity varies with the isotopic composition of the sample. Many current neutron scattering methods are not themselves new, but modern experiments are being made more powerful by rigorous coupling to computational simulations and by having more intense neutron sources. This allows for a much-improved interpretation and deconvolution of the experimental data, as well as serving to improve the confidence and extensibility of the simulation. Moving forward, neutron scattering will remain a key to understanding geochemical phenomena, especially as more advanced techniques are developed. These include more accurate and large-scale simulation capabilities (e.g., machine-learning parameterized atomic

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REFERENCES


Liquids, glasses, and amorphous materials are ubiquitous in the Earth sciences and are intrinsic to a plethora of geological processes, ranging from volcanic activity, deep Earth melting events, metasomatic processes, frictional melting (pseudotachylites), lightning strikes (fulgurites), impact melting (tektites), hydrothermal activity, aqueous solution geochemistry, and the formation of dense high-pressure structures. However, liquids and glassy materials lack the long-range order that characterizes crystalline materials, and studies of their structure require a different approach to that of conventional crystallography. The pair distribution function is the neutron diffraction technique used to characterize liquid and amorphous states. When combined with atomistic models, neutron diffraction techniques can determine the properties and behavior of disordered structures.

**THE DISORDERED STATE**

Water and silica represent two of the most abundant compounds on Earth and are commonly encountered as liquids, or in amorphous or glassy forms. The structure of clathrates and aqueous solutions, for example, are defined by their hydrogen-bonding arrangements and the formation of solvation shells. Amorphous calcium carbonate (the least stable form and the one found in the shells of sea urchins, mollusks, corals, as well as a component of tufa) and other amorphous materials can be formed by a variety of different mechanisms. Refractory liquids, such as silicates, which are the focus of this article and which require access to high temperatures and pressures to study, have a strong glass-forming ability (or fragility), and melt equivalents are often studied in the glassy state (Hannon 2015). Unlike crystalline phases, liquids, glasses, and amorphous materials can encompass a vast range of compositions, and the local structure—defined by the coordination number—plays a crucial role in determining their properties and behavior. Liquid structures can be directly associated with many thermodynamic and physical properties, including density, heat capacity, thermal expansion, diffusion, and viscosity (Fig. 1) (Poirier 2000). Of these, density is the most directly connected to structure. To help understand these relationships, it is useful to classify liquids according to the nature of the interatomic forces that govern their structure: for example, there are spherical molecules (Ar), diatomic molecules (H₂), metals (Fe), molten salts (NaCl), covalent liquids (SiO₂), and hydrogen-bonded liquids (H₂O) (Egelstaff 1994). Neutron scattering provides a direct probe of the interatomic forces in these liquids and provides a stringent test of atomistic models and properties predicted from these models. Total neutron scattering, conventionally presented as the pair distribution function (PDF), can provide insight on the atomic-to-nanometer scales and provides answers to many geologically important questions related to physical properties. For example, how many gas molecules can be confined in a clathrate hydrate and what is the shape of the clathrate? How does calcium carbonate form, and what are the reaction pathways that can be followed? Or, in the case of silicate liquids, what determines if the melt cools to form a crystalline or glassy phase?
NEUTRON SCATTERING AND THE PAIR DISTRIBUTION FUNCTION (PDF)

Neutron scattering studies of liquids and amorphous materials have a long history, with the main quantity of interest being the extraction of an accurate PDF against which structural models can be rigorously tested. The quantity measured, however, is a scattered intensity (S) as a function of scattering angle and/or neutron wavelength, which is converted to momentum transfer (Q) (see Ross and Cole 2021 this issue). Disordered materials scatter neutrons diffusely, and detectors placed at fixed angles measure the scattered intensity. Great care is taken to design neutron experiments so that accurate normalization and correction procedures can be applied to the diffusely scattered data and extract the scattered intensity. Neutrons have the advantage over X-rays that a sample of vanadium in the same size and geometry as the material of interest can be used to normalize the scattering data on an absolute scale. Separation of the coherent scattering resulting from the interference between different atoms yields the total structure factor, which is directly related to the total PDF through a sine Fourier transform.

The PDF describes the probability of finding an atom at a given distance from an atom at the origin, averaged over all the atom–atom correlations in the entire liquid (Fig. 2). The area under the peaks in a PDF can be related to the coordination number. For a monoatomic system, it is straightforward to relate the measured PDF to theory and, particularly, the bonding forces between atom pairs. Here, the location of the first maximum in the PDF corresponds to the average nearest neighbor atom–atom spacing, and the closest approach between atoms is defined by the repulsive forces between them.

Although the study of mono-atomic liquids, particularly at extremes of pressure and temperature, is a rich area of research, liquids of geological interest are inherently multicomponent. Taking the example of high-temperature silicate melts, the local and intermediate-range structures have a strong influence on viscosity and thermodynamic properties and have been of long-standing interest in Earth and glass science (Wilding and Benmore 2006). For these multicomponent systems the total structure factor and transformed real space PDF is the weighted sum of all the partial atom–atom pair contributions. For a system of n atom types there are n(n + 1)/2 partial contributions. So, for SiO2 there are three partial contributions: Si–O, Si–Si and O–O. The addition of a modifier such as Na2O increases number of partial PDFs to 6 and so on. For chemically complex systems the task of extracting meaningful information is problematic without significant modeling efforts or additional information from other techniques, such as high-energy X-ray diffraction or nuclear magnetic resonance. Complementary neutron and X-ray PDF techniques are commonly applied to liquids, glasses, and amorphous materials to extract partial PDFs (Fischer et al. 2006).

NEUTRON DIFFRACTION WITH ISOTOPIC SUBSTITUTION (NDIS)

The fact that neutrons scatter from nuclei, rather than from electrons, means that access to high momentum transfer is possible without the loss of signal due to the electron charge distribution which is intrinsic to X-ray diffraction. High-Q measurements lead to high-resolution PDFs, in which precise bond lengths and a better separation of atom–atom correlations are obtainable. Nevertheless, the most sophisticated neutron technique associated with PDF measurements is the application of the isotopic substitution technique, albeit limited to only certain elements (nuclides) (Table 1) (see Ross and Cole 2021 this issue). Neutron diffraction with isotopic substitution (NDIS) uses chemically identical samples, differing only in the isotopic enrichment of one component. The method relies on the peculiar feature that for some isotopes the scattering length can be negative, meaning that different atom–atom correlations involving that isotope appear as negative dips in the PDF rather than as positive peaks. One important example is that of hydrogen–oxygen correlations. The correlations of O–H in H2O are negative whereas the O–D correlations in D2O are positive. The H/D substitution is a very important tool in the study of aqueous and other hydrogenous liquids (Soper 2001). Ultimately, however, it is the difference between chemically identical but isotopically different samples that provide the most detailed information. The first two rows in Table 1 illustrate the most suitable elements for isotopic substitution in silicate liquids; Figure 3 shows a typical binary oxide phase diagram with different size atoms depicting the different neutron cross sections of the Ca–O polyhedra in CaO–SiO2.
Elements with isotopes suitable for neutron diffraction with isotopic substitution (NDIS) experiments; $\Delta b$ is the maximum difference in coherent scattering lengths between isotopes; fm = femtometer.

<table>
<thead>
<tr>
<th>Feasibility of NDIS experiments</th>
<th>Elements with naturally occurring nuclides</th>
</tr>
</thead>
<tbody>
<tr>
<td>Second order difference $\Delta b &gt; 10$ fm</td>
<td>H, Ar, Ti, Ni, Hf, Ag, Sm, Dy, Yb</td>
</tr>
<tr>
<td>First order difference $\Delta b &gt; 1$ fm</td>
<td>Ce, Cu, Zn, Ga, Ge, Se, Si, Zr, Mo, Pb, Ag, In, Te, Ba, W, Os, Pt, Ti, Ce, Nd, Eu, Gd, Er, Lu</td>
</tr>
<tr>
<td>Feasible</td>
<td>O, Si, Rb, Sn, Sb, Re, Pb</td>
</tr>
<tr>
<td>To be determined</td>
<td>Br, K, Ru, Xe, La, Ta, Ir</td>
</tr>
</tbody>
</table>

RANGES OF ORDER

Even in liquids and glasses there are different ranges of order to be considered, which can be associated with different structures within the PDF. For example, in the archetypical glass-forming system SiO$_2$ at ambient pressure, the first true peak in the PDF corresponds to the shortest bond distance ($R_{O-O}$). This is followed by the O–O peak associated with SiO$_4$ tetrahedra, where $R_{O-O} = \sqrt{8}/3 R_{Si-O}$ for perfect tetrahedra. The first few peaks in the PDF, therefore, define the local structural units. The area under each of these partial PDF peaks is directly related to their coordination numbers, i.e., the number of O atoms around Si is 4 in silica under ambient conditions, and, conversely, the number of Si atoms around O is 2. At longer distances, the Si–Si correlation appears between adjacent tetrahedra (Fig. 2) which is related to the Si–O–Si bond angle distribution and contains information about the connectivity between polyhedra. A series of corner-shared SiO$_4$ tetrahedra can link to form different-sized rings. Arrangements of these structures can lead to intermediate-range ordering within a glass or liquid.

As illustrated in Figures 2 and 3, neutrons are sensitive to the locations of oxygen atoms. For more complex systems, the local oxygen coordination can give an indication of the formation of oxygen triclusters. Oxygen triclusters indicate the presence of a dense structure with very little network formation or void space. For multicomponent systems, the integrated areas under overlapping peaks beyond the first shell can be difficult to determine, and chemical constraints or additional information from other experimental techniques are essential for an accurate interpretation. The peak positions in the 3–5 Å region in the PDF are often compared to known crystal structures, to identify edge-sharing and corner-sharing ratios between adjacent polyhedra. Readily available atomistic modeling or simulation methods are required to extract bond-angle distributions and ring structure statistics consistent with the PDF data. The intermediate-range order associated with the ring distributions in network-forming silicates is contained in the prominent peak in the total structure factor at the lowest Q value: this is referred to as the “first sharp diffraction peak” (FSDP). Models of ring statistics or intermediate-range order due to 1-D chains, 2-D sheets, or 3-D networks can often be more readily tested by comparing them to the FSDP rather than to the PDF. Here, the position of the FSDP indicates ordering in real space with a periodicity of $d = 2\pi/ Q_s$, where $Q_s - r_1 - 2.5$, and $r_1$ is the position of the first peak in the PDF (Price et al. 1989). However, not all glasses exhibit a peak at this location and, due to unfortunate terminology, the FSDP is often mistaken for the second sharp diffraction peak or principal peak in S(Q).

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High-pressure diffraction studies generally show a decrease in the FSDP intensity and an increase in height of the principal peak as ring structures collapse and chemical ordering increases. Element-specific coordination numbers have been obtained through the extraction of partial structure factors for glassy SiO$_2$, measured using a combination of NDIS using Si and high-energy X-ray diffraction (Mei et al. 2008).

Theory, modeling, and simulation techniques have always been closely linked to the interpretation of neutron PDF experiments on liquids and glasses and are well-established in the disordered materials community. Reverse Monte Carlo methods (McGreevy 2001) and empirical potential structure refinement modeling methods (Soper 2001) have been developed to provide atomistic or molecular models to be in perfect agreement with diffraction data based on local chemical and density constraints. Figure 4 illustrates this approach as applied to neutron diffraction data obtained for a forsterite (Mg$_2$SiO$_4$) composition glass. At the other end of the spectrum, the neutron PDF is directly comparable to ab initio molecular dynamics simulations and density functional theory calculations. More commonly, for oxides, classical molecular dynamics simulations and the development of interatomic pair potentials are used to interpret the basic mechanisms behind geological processes and behavior.

**NEUTRON INSTRUMENTATION AND SAMPLE ENVIRONMENTS**

Direct geometry total scattering diffractometers, which can study of liquids and glasses, take advantage of high neutron energies to access high Q values, which in turn leads to high resolution in real space. Because the intensity of the scattered signal from disordered materials is diffuse, the signal/noise ratio is important and Q-space resolution is often sacrificed for flux on PDF instruments to maximize the counting statistics. There are two main types of neutron source: 1) steady state reactor source; 2) pulsed spallation source (Windsor 1981; Ross and Cole 2021 this issue).

Neutron experiments typically require large volumes (~cm$^3$) of material. Glassy and amorphous materials can be contained in cylindrical thin-walled vanadium foil cans because the incoherent (single atom) scattering of...
vanadium makes the container signal essentially flatline. For solutions that can react with vanadium, the “null scattering” (a balance between positive and negative scattering lengths) Ti₅₂Zr₄₈ alloy is often used. Most geologically important processes involving liquid silicates occur at high pressures or high temperatures (usually both), and these structures are not always easily recovered, so the study of liquids in situ at these extreme conditions is desirable. Specialized sample environments have been developed for ambient-pressure studies of high-temperature silicate liquids and ambient-temperature high-pressure neutron diffraction studies of silicate glasses.

Existing furnaces used for liquid studies at neutron sources only have maximum operating temperatures of ~1,100 °C, which are below the melting points of many silicate liquids. Furthermore, the scattering from bulky, polycrystalline furnaces would dominate the signal over that of the weakly scattering liquid, making extraction of an accurate PDF problematic. An alternative approach is to eliminate the container completely. Over the past few decades, there have been an increasing number of neutron diffraction experiments of liquids using containerless techniques. To attain temperatures of >1,500 °C, the aerodynamic levitation furnace (Fig. 5) can be used to study oxides. This furnace comprises a water-cooled conical nozzle in which a small bead of material (2–3 mm in diameter) is levitated by a few hundred microns using a gas jet of argon or air. The bead is heated from above by a high-powered CO₂ laser. This enables a variety of liquids to be studied over a wide range of temperatures, up to ~2,700 °C, and, despite the small sample size, liquid diffraction experiments have become feasible at high-flux neutron sources (Benmore and Weber 2017). Recent developments have shown that with the introduction of gas mixing (CO/CO₂) there is the potential to study mixed valence liquids, most importantly iron, over a range of oxygen partial pressures. The absence of heterogeneous nucleation sites means that containerless techniques can be used to explore deep supercooled liquids several hundred degrees below the melting point (Shi et al. 2019), which is particularly important for fragile liquids where the structures of the liquids are expected to change significantly in the metastable regime. The most frequently used high-pressure sample environment for neutron scattering is the toroidal, opposed-anvil device, usually referred to as the Paris–Edinburgh cell (Chakoumakos and Parise 2021 this issue). This was developed specifically for high-pressure neutron crystallography but has been adapted for total scattering studies of glasses. Extracting the total neutron structure factor for a glass at high pressure is challenging. The difficulty arises from the background contributions from the cell itself, which are pressure-dependent, and from deformation of the gasket with pressure, which changes the attenuation path of the neutrons. At the high-pressure PLANET beamline (at the Japan Proton Accelerator Research Complex), a purpose-built six-axis multi-anvil press has been developed that uses two-stage anvils. In this case, the incident neutron beam is directed through a gap between the anvils, and scattered neutrons emerge at right angles to the incident beam with radial collimation to remove parasitic Bragg peak contributions from the high-pressure assembly. The feasibility of using the six-axis multi-anvil cell configuration for probing amorphous materials has been demonstrated by a measurement of SiO₂ glass at a pressure of 9.4 GPa with a total structure factor obtained to a Q value of ~30 Å⁻¹ (Hattori et al. 2015). Experimental corrections can be evaluated by using suitable pellets of vanadium to determine the background contributions under load. Recent developments using large-volume diamond anvil cells for neutron diffraction on the Spallation Neutrons and Pressure beamline (at the Spallation Neutrons Source facility at Oak Ridge, Tennessee, USA) have achieved considerably higher pressures of ~100 GPa for samples of ~0.05 mm³ (Tulk et al. 2019). The extraction of reliable total structure factors at such extreme pressures would represent a major advancement for the PDF technique.

**EXAMPLE GLASS AND LIQUID SILICATE SYSTEMS PROBED BY NEUTRONS**

Many liquids of interest in the Earth sciences are complex silicates. Glasses and liquids formed in the SiO₂ system are modified by the addition of cations, such as alkali or alkaline earth elements with other components such as A₂O₅. The SiO₂ framework becomes disrupted by the incorporation of modifying cations, causing the formation of nonbridging oxygens. These “network modifier” cations tend to cluster rather than disperse randomly throughout the structure. These modified random networks form the basis for any model of a geologically relevant glassy silicate; density, viscosity, or fragility are often systematically studied as a function of composition. Alkali silicate glasses produced by conventional methods have been studied for decades, and when more than one alkali modifies the silicate network then liquid and glass structures can
Neutron diffraction studies on silicate liquids and is a favorable element for isotopic substitution measurements (Table 1). Neutron diffraction experiments combined with atomistic simulations have shown that ferric iron is predominantly four-coordinated in sodium silicates (Weigel et al. 2008) and that both ferrous and ferric iron also exist in a 5-fold medium-range ordering. For example, Ca and Mg have been shown to mix randomly, whereas mixtures of K and Mg show medium-range ordering. The effect of mixing alkalis on medium-range ordering has also been investigated using neutron diffraction experiments combined with atomistic simulations, finding a reduction in the size of cavities within the network due to K–Na pairing in the interstitial space associated with nonbridging oxygens (Onodera et al. 2019).

Iron is an important component in naturally occurring silicate liquids and is a favorable element for isotopic substitution measurements (Table 1). Neutron diffraction studies have shown that ferric iron is predominantly four-coordinated by oxygen in sodium silicates (Weigel et al. 2008) and that both ferrous and ferric iron also exist in a 5-fold coordinated local environment with no six-coordinate iron present. This study also indicates that iron is heterogeneously distributed throughout the silicate network. Traditionally, 4-fold tetrahedra are viewed as network forming, and 5-fold and 6-fold polyhedra as network modifying. Calcium and magnesium also represent modifiers suitable for NDIS experiments and have often been used as benchmark systems for testing theories of modifier ordering. Measurements from NDIS have shown a high degree of intermediate-range ordering in calcium silicate glasses, persisting up to 1 nm (Gaskell et al. 1991). Calcium silicate liquids are good candidate systems for levitation and are less susceptible to evaporation over the extended periods of heating required for a neutron experiment. A neutron diffraction study on a levitated calcium silicate liquid using isotopic substitution coupled with molecular dynamic simulation demonstrated significant differences between the liquid and glassy state of this moderately fragile liquid (Skinner et al. 2012). The liquid structure was found to be characterized by short chains of edge-shared CaO₆ octahedra and a more distorted Ca–O local environment than in the glass.

In addition to the opportunities offered for in situ studies, containerless techniques can be used to produce exotic glasses not easily fabricated by other methods. Glasses produced using an aerodynamic levitation furnace in the MgO–SiO₂ system, between the compositions of the peridotite components MgSiO₃ and Mg₂SiO₄, are used to approximate liquids produced within the Earth’s mantle. Neutron experiments on MgO–SiO₂ glasses combined with X-ray diffraction and computer modeling reveal a distribution of MgO₄ polyhedra that are heterogeneously distributed within the silicate matrix and show that the Mg–O coordination numbers are significantly lower than for the crystalline phases. There is a change in structure from silicate chains in the more silica-rich compositions to a Mg network at the MgSiO₄ composition. The latter composition is on the limit of glass formation in the system: edge-shared MgO₆ polyhedra form a continuous network, whereas the silicate component is restricted to isolated SiO₄ tetrahedra and Si₂O₆ dimers (Cormier and Cuello 2011; Kohara et al. 2011). Figure 4 shows the results of a reverse Monte Carlo fit to neutron diffraction data obtained from a forsterite composition glass produced by containerless techniques. However, in situ experiments are required for a true understanding of structure and viscosity under the high temperatures and pressures of the Earth’s mantle. High-pressure neutron studies on glassy CaSiO₃ and MgSiO₃ show an increase in cation coordination number accompanied by an increased fraction of cation-bridging oxygen bonds, although high-pressure neutron studies on the corresponding melts have yet to be performed.

When vitreous SiO₂ is compressed there is significant breakdown in the degree of intermediate-range order, which is shown by a decrease in the height of the FSDP (Zeidler et al. 2014) and which leads to a collapse of the void space formed by the corner-linked tetrahedra in the network. This is reflected as the change in bond angle between adjacent silicate tetrahedra and a corresponding change in sound velocity, determined by ultrasonic or Brillouin scattering measurements. At higher pressures (>10 GPa), the population of higher coordinated silica increases, and further densification results through edge-sharing of five- and six-coordinate silicon. Water is the most important volatile element in silicate liquids, its presence strongly influences liquid viscosity and its exsolution controls such processes as the style of a volcanic eruption. Water reacts with the silicate network to form hydroxyl species which disrupt SiO₄–SiO₄ linkages. Significant amounts of water can be dissolved in silicate glass, and there can be both molecular water and hydroxyl species present. A neutron diffraction study of pure silica glass with 13 wt% D₂O synthesized under high-pressure–high-temperature conditions was performed by Urakawa et al. (2020). The addition of water disrupted the silicate network to form water-rich regions of less than 100 Å, shifting the FSDP to higher Q and reducing the ring-size distribution (Fig. 4). At high pressures and high temperatures, water and SiO₂ become completely miscible. The pressures and temperatures required for the formation of these hydrous fluids is close to the limit of feasibility of current sample environments, although quasi-elastic neutron scattering to investigate proton dynamics has been achieved (Yang et al. 2017). Preliminary studies to explore the SiO₂–D₂O system at high pressure and high temperature demonstrated the formation

**Figure 5** (top) A gas jet is used to levitate a high-temperature silicate bead during and after melting. (bottom) A schematic of the associated aerodynamic levitator instrumentation integrated into a neutron beamline.
of the fluid. However, the contribution from the tungsten carbide anvils overwhelms the signal and prevents a quantitative structure factor from being extracted.

PROSPECTS

In 1994, Prof. Adrian C. Wright (Reading University, UK) published his seminal article “Neutron Scattering from Vitreous Silica: What Have we Learned from 60 Years of Diffraction Studies?” (Wright 1994), in which the structure of SiO₂ glass at ambient conditions was discussed in detail. In 1994, after 87 years of diffraction studies, much progress has been made in the field of melts, glasses, and amorphous materials through the construction of intense neutron sources and from major strides in atomistic modeling and simulation methods. Yet more is on the horizon. The advent of high-flux neutron sources combined with innovative large diamond anvil cells shows much promise for high-pressure studies on glassy and amorphous materials up to and above 25 GPa (Guthrie 2015). Lower pressure and high-temperature studies on hydrous silicates, hydrothermal fluids, and low-pressure–low-temperature studies of clathrate formation also represent areas of great potential that are ideally suited to neutron scattering studies. At spallation neutron sources, levitation experiments with neutron time stamping have demonstrated the capability of repeatedly cycling laser heating/cooling ramps to build up statistics and investigate the in situ formation of metastable phases and glass formation (Shi et al. 2019). These in situ studies offer the potential to explore a wide parameter space and are particularly well-suited to geologically relevant liquids: the influence of composition, temperature, and fugacity could be explored. Such experiments are particularly well-suited to iron-bearing systems, which have suitable isotopes for NDIS experiments. Finally, we return to the point made at the outset, the fact that there is a direct fundamental relationship between practical neutron scattering data from liquids and theoretical investigations. With this in mind, combining small- and wide-angle neutron scattering to span both atomic and mesoscopic length-scales and obtain extended-range PDFs is already underway (Bowron et al. 2010). This coincides with parallel efforts to use machine learning on supercomputers to predict the structure of liquid, glassy, and amorphous materials on large simulation cells with ab initio accuracy (Sivaraman et al. 2020).

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The development of sophisticated sample environments to control temperature, pressure, and magnetic field has grown in parallel with neutron source and instrumentation development. High-pressure apparatus, with high- and low-temperature capability, novel designs for diamond cells, and large volume presses are matched with next-generation neutron sources and moderator designs to provide unprecedented neutron beam brightness. Recent developments in sample environments are expanding the pressure–temperature space accessible to neutron scattering experiments. Researchers are using new capabilities and an increased understanding of the fundamentals of structural and magnetic transitions to explore new territories, including hydrogenous minerals (e.g., ices and hydrates) and magnetic structural phase diagrams.

**INTRODUCTION**

Phase transitions, whether structural or magnetic, involve symmetry breaking, and symmetry analysis methods provide powerful tools to follow the atomic or spin structural changes. Neutron scattering offers both unique and complementary tools for studying phase transitions in minerals. Neutrons are unique in the sense that they have a magnetic moment that scatters from the magnetic ions in materials, and the use of spin-polarized neutron beams can separate magnetic from nuclear scattering, making neutron diffraction the method of choice for determining magnetic structures.

Neutron studies of phase transitions complement studies using X-rays in the sense that neutrons scatter from the atomic nuclei. This means that they can offer greater fidelity than X-rays in distinguishing light elements in the presence of heavy elements, distinguishing neighboring elements in the periodic table, and even distinguishing between isotopes of the same element. Neutron diffraction or neutron elastic scattering methods reveal structural details, while inelastic neutron scattering methods probe the dynamical picture and can unlock the origins of phase transitions by following changes in phonons. Neutron diffraction has made significant contributions to understanding materials that are largely hydrogenous (e.g., water ices, clathrate hydrates) or for which oxygen or other relatively light elements have the most significant displacements.

In this context, we introduce recent developments in design and in the deployment of sample environments for neutron experiments that are used to induce phase transitions in minerals, and we discuss what can be learned about phase transitions, including magnetic ordering, in mineralogical materials using neutron scattering. Phase transitions often involve distortions of the parent mineral structure due to one or more combinations of lattice strains, atomic displacements, magnetic moment ordering, or chemical ordering in crystallographic sites. Neutron scattering methods contribute towards two goals in the study of phase transitions: 1) to characterize them experimentally by determining the transition temperature, pressure, or field, and the associated structural and dynamical changes; 2) to understand the driving mechanism of a given transition (Redfern and Harrison 2009). The former is dominated by elastic scattering methods (e.g., diffraction; neutrons scattered without changing energy due to interaction with the sample), whereas the latter is dominated by inelastic scattering methods (scattering processes whereby the neutron’s energy is transferred to or from the sample). We will limit the scope to the elastic scattering methods. The study of minerals from this perspective offers a greater understanding of mineralogy, petrology, and geochemistry, and also significantly informs materials science and technology.

**SAMPLE ENVIRONMENTS**

Because neutrons are neutral particles, they penetrate most structural materials deeply, facilitating the design of complex sample environments (Bailey 2003) that simulate real-world physical conditions. High pressure (HP) is of great interest to the mineralogical community, especially when paired with simultaneous high temperature (HT), because most Earth materials operate under conditions of HP-HT. Increasingly, however, there is interest in simulating materials on icy planets and moons via analogue studies of materials at simultaneous HP and low temperature (LT). Many decades of development have produced a number of “standard” sample environments, which have been described in detail (Bailey 2003). Most neutron user facilities maintain a sample environment group to continue developing new devices and to curate legacy equipment.
For example, the Neutron Science Division at the Oak Ridge National Laboratory (Tennessee, USA) maintains a catalog of sample environments (https://neutrons.ornl.gov/sample) for its reactor neutron source (the High Flux Isotope Reactor) and spallation neutron source (the Spallation Neutron Source). “Standard” equipment available worldwide includes the so-called orange cryostat, which was developed at the Institut Laue–Langevin (Grenoble, France) in the 1970s for continuous operation between 1.5 K and 300 K, and since copied at most reactor and spallation sources (Bailey 2003). For HT studies, wound furnaces are available in many configurations (vacuum, gas controlled) up to 1,600°C. Levitation techniques allow for samples to be laser heated up to 2,700°C without the need for a container, increasing signal-to-noise discrimination for studies of liquids, while varying fugacity (see Benmore and Wilding 2021 this issue).

**PRESSURE CELLS**

Various pressure cells have been optimized for neutron scattering, enabling different sample types (powder vs. single-crystal; large vs. small volume), different measurement types (diffraction, small-angle scattering, inelastic scattering), and a variety of pressure–temperature conditions to be accessed (Fig. 1). Gas cells find most use with diffraction and small-angle scattering but have limited pressure ranges, generally below 0.6 GPa, with combined low- and sometimes modest temperatures of a few hundred degrees.

For studies above 1 GPa, the Paris–Edinburgh cell (Besson et al. 1992) is the most widely used large-volume HP cell at both spallation and reactor neutron sources for powdered samples. The Paris–Edinburgh cell can approach 30 GPa using specialized anvils, it allows pressure changes in situ, it can be cooled to 85 K, and it can be heated to hundreds of degrees, but with much lower combined pressure. For single-crystal studies below 2 GPa, finger-size clamp cells are better suited because they can be cooled to ultralow temperatures and, for some designs, can accommodate combined high magnetic fields. The main drawback of clamp cells is that the pressure must be changed ex situ. Of the different cell types, the Paris–Edinburgh cell has had the most use in geologically relevant studies, e.g., extensive studies of ices (see Klotz et al. 2002 and references therein).

**Diamond Anvil Cells**

Diamond, and other “gem cells”, have also been adapted for use with neutron scattering, chiefly by overcoming previous limitations imposed by the source and the need for large sample volumes. Most of the disadvantages of gem cells are now offset with the development of higher brightness moderated neutron sources, detectors of greater sensitivity, and tougher multicaret chemical vapor deposition–grown diamond anvils (Fig. 1). Recent experimental results suggest a new generation of diamond anvil cell, one designed for neutron sources and which holds great promise for diffraction studies of single crystals and powders, especially when coupled to focusing optics and sensitive area detectors.

Boehler et al. (2013) introduced the first diamond anvil cell designed specifically to take advantage of the area detectors installed at the Spallation Neutrons and Pressure (SNAP) beamline at Oak Ridge National Laboratory’s Spallation Neutron Source. The cell uses a conical anvil design which strongly supports the chemical vapor deposition–grown diamond anvils (Fig. 2). By using 1.0 mm beveled diamond culets, pressures of 94 GPa have been achieved, and high-quality neutron powder diffraction data have been obtained on ice for a pressure regime not previously accessible to neutron techniques (Guthrie et al. 2013). Development of the so-called neutron diamond anvil cell has proceeded rapidly (Haberl et al. 2019), with applications to highly precise single crystal and powder diffraction studies using several diffractometers at the Oak Ridge National Laboratory’s Spallation Neutron Source and High Flux Isotope Reactor. The neutron diamond anvil cell has also been used at the Oak Ridge National Laboratory Spallation Neutron Source’s VISION spectrometer to do vibrational spectroscopy.

**Figure 1** A selection of neutron high-pressure sample cells that cover the pressure–temperature ranges shown in the labeled shaded areas on the graph. (A) ATSUHIME large volume six-anvil device installed at J-PARC (Japan). (B) The Paris–Edinburgh cell, which is available at many neutron sources. (C) The multicaret chemical vapor deposition neutron diamond anvil cell, which can have a selection of anvils (shown above it); the one illustrated is operational at the Oak Ridge National Laboratory (Tennessee, USA). The diagonal line is an approximate geotherm. Abbreviation: RT = room temperature. The points indicated by 77 (N$_2$) and 4 (He) represent liquid nitrogen and liquid helium temperatures in Kelvin. After Hattori et al. (2015).
Multi-Anvil Devices
At J-PARC (Japan), the HP community’s innovation in designing multi-anvil HP devices and interfacing them to X-ray beamlines has been harnessed in the design of the multipurpose PLANET facility (Hattori et al. 2015), anchored by the six-axis press known as ATSUHIME (Fig. 3) which was designed for time-of-flight powder neutron diffraction. The ATSUHIME instrument is the first multi-anvil press installed at a large neutron user facility that is intended for mineral studies under HT and HP into the 14 GPa and 2,000 K range relevant to the bottom of the upper mantle (Fig. 1). It is used on a broad range of problems in physics, chemistry, and planetary sciences.

Neutron studies of H(Don)-bonded networks began almost as soon as reliable neutron sources became available (Pepinsky 1954) and the issue of hydrogen bonding “centering”, where the proton is induced to be equidistant between acceptor and donor oxygens, was an early and lasting fascination (Ellison and Levy 1965). Centering was initially induced chemically, and it became clear early on that pressure provides a clean isochemical route to study the relationship between hydrogen bonding, the competition between H⋯H repulsion and disorder, and sample volume. Depending on temperature and pressure, water solidifies in several crystalline and amorphous forms. The incorporation of small molecule “guests” confined in a “host” lattice consisting of water adds greater structural complexity in materials known as clathrate hydrates. The nomenclature for these clathrates follows the form sT where “s” denotes “structure” and T denotes the “type”; thus sII, structure type II. A recently discovered unique structure, based on spiral channels rather than cages, is designated sX, “structure X” to distinguish it from previously described cubic (sI and sII) and hexagonal (sH) clathrate hydrates (Massani et al. 2019). The clathrate designated sX illustrates the richness and pathway dependence of new phenomena in ices at low pressures. The sX type of structure is chiral, with channels rather than cages, and is not based on a stable ice structure, silica polymorph, or zeolite. The sX structure is known to form from hydrogen–water and carbon dioxide–water mixtures at pressures above 0.3 GPa and at temperatures between 77 K and 195 K. Massani et al. (2019) show that sX is also refillable with nitrogen, after being produced by elimination of hydrogen, and with the guest:host ratio of ~2.5. Analysis of neutron powder diffraction data also show that, during decomposition, nitrogen-filled sX undergoes several transitions into the exotic hydrates sH and sIII—not observed at these pressure–temperature conditions—before forming the stable nitrogen hydrate sII. More recently, Fortes et al. (2017) combined HP neutron powder diffraction (Paris–Edinburgh cell) and quasi-elastic neutron spectroscopy (gas cell) to study the phase behavior and compression mechanism for the deuterated analogue of meridianite, MgSO₄·11D₂O, which is a candidate rock-forming mineral in some icy satellites and, possibly, in the polar regions of Mars. Measurements in the range 0.1 < P < 800 MPa and 150 < T < 280 K were carried out at the PEARL instrument of the ISIS Neutron and Muon Source facility (Rutherford Appleton Laboratory, UK), while simultaneous elastic and quasi-elastic measurements were carried out up to 550 MPa using the OSIRIS spectrometer. Diffraction measurements revealed the most compressible
direction was perpendicular to the long axis of a discrete hexadecameric water cluster, \( (D_2O)_n \). Phase transitions at 545 MPa/275 K were attributed to peritectic melting, and at 0.9 GPa/240 K to decomposition into HI water ice phase VI and MgSO\(_4\)-9D_2O; the latter phase had only previously been reported as forming at ambient pressure by quenching small droplets of MgSO\(_4\)aq in liquid nitrogen. The OSIRIS quasielastic neutron spectra indicate the onset of the reorientation motion of D_2O molecules with characteristic timescales of 20–30 ps, commensurate with the lifetime of solvent-separated ion pairs in aqueous MgSO\(_4\).

Mineral physics applications of the neutron diamond anvil cell are only now getting underway in earnest. Opportunities abound, given that both single-crystal and powder samples can be used and that the cells can be gas-loaded, cooled, or (laser) heated. Recent examples are the investigation of hydrogen-bond geometries in potassium dideuterium phosphate and in ice VI, determined as a function of pressure (Massani et al. 2020).

A good example of the science being produced using the multi-anvil press ATSUHIME is powder neutron diffraction of the decomposition mechanism of the hydrogrossular mineral katoite [Ca\(_3\)Al\(_2\)(O\(_2\)D\(_4\)]. At 9 GPa, the diffraction results show that HP increases the dehydration temperature of katoite from 300 °C to 900 °C. The data were of sufficient quality to indicate the relative compressibility of polyhedra in hydrogarnet: at 8 GPa and up to 850 °C, the volume of the CaO\(_8\) dodecahedron expands by about 8% and that of the AlO\(_6\) octahedron by about 13%, while the tetrahedra contract by about 10%. Interestingly, Kyono et al. (2019) observe the O–D bond distance shrinking just before decomposition and posit that this shortening is caused by D–D repulsion, which destabilizes the O–D bond and so leads to the thermal decomposition of katoite. Detailed studies such as this help to understand what structural bonding motifs can persist to high pressures, and how they evolve with pressure.

**MAGNETIC PHASE TRANSITIONS**

Two important interactions occur in the scattering of neutrons by atoms: the short-range nuclear interaction of the neutron with the atomic nucleus, and the interaction of the neutron’s magnetic moment with the magnetic moment of unpaired electrons in the atom. Both of these can be of equal magnitude and are simply combined (are additive) in the scattering pattern. Atoms with unpaired outer electrons are typically transition metals, lanthanides, and actinides. The magnetic scattering decays with scattering angle much like X-ray scattering does, but even more rapidly because the electrons are in the outer shells. Consequently, magnetic scattering is observed at low scattering angles.

In their seminal work, Shull and Smart (1949) experimentally demonstrated the Néel theory of antiferromagnetism in MnO, constituting the very first magnetic structure determination using neutron diffraction. The antiparallel alignment of adjacent magnetic moments on the manganese ions results in the magnetic unit cell doubling in size in each direction as compared to the chemical unit cell, giving rise to extra (superlattice) magnetic-only reflections in the diffraction pattern (Fig. 4). In addition, the intensities of the magnetic peaks were investigated below the ordering temperature and these magnetic peaks became saturated as the Mn\(^{2+}\) moments became fully ordered. Thus, the transition from the paramagnetic to the antiferromagnetic state was mapped using neutron diffraction.

Recently, the combined pressure and temperature dependence of the Mn magnetic moment and the rhombohedral distortion in MnO were determined by neutron powder diffraction (Klotz et al. 2020). The onset temperatures for both magnetic ordering and rhombohedral distortion tend to shift upward with pressure, suggesting the distortion is fully due to the magnetic ordering. Complementary X-ray-diffraction measurements show that even at 295 K and 42 GPa, MnO is thorouglyly distorted, and, hence, magnetically ordered.

Historically, magnetic structure has been determined largely by trial-and-error solutions to best-fit measured neutron diffraction peak intensities, the models often being guided by complementary information such as magnetization measurements. Nowadays, symmetry analysis methods, such as group theory, have overwhelmingly replaced trial-and-error. Symmetry analysis defines possible models, allows for a more complete appraisal of all possible solutions, and identifies which symmetry modes are possibly involved in the transition. The majority of magnetic structures are determined by neutron diffraction, mostly using powders and, to a lesser extent, using single crystals, the latter being better at unequivocally identifying the correct solution. Optional enhancements, such as polarized neutron diffraction, are used to unambiguously separate the magnetic from the nuclear scattering: nuclear scattering preserves the spin state of the incoming neutrons, whereas magnetic scattering can cause the spin state to flip, meaning that detecting the spin-flip intensity can allow the magnetic scattering to be separated from the nuclear scattering. This is crucial in some cases, particularly for ferromagnetic materials for which the magnetic peaks wholly coincide with the nuclear peaks (see Ressouche 2014 for an overview of polarized neutron diffraction methods and applications). In addition to the temperature control necessary to record data above and below the magnetic ordering temperature, an applied magnetic field also can be used to align moments in a particular direction and to explore magnetic phase diagrams as a function of magnetic field. High-field magnets developed for this purpose are usually used in combination with low temperatures. Analogous to chemical structures, magnetic structures also change as a function of temperature, pressure, chemical solid solution, and even crystallite size (think nanoparticles).

Interest in magnetic structures is greater than ever, and the number of neutron powder and single-crystal diffractometers available to researchers now are also greater than at any time in history. As a consequence, the number and complexity of the magnetic structures now determined is growing rapidly, primarily driven by interests in materials physics and chemistry. Geoscientists, given the user-friendly resources and analysis tools, are now also showing more interest and wanting to study the magnetic structures of minerals, recognizing not only that magnetic structural phase diagrams are fundamental to planetary paleomagnetism but that the mineral kingdom offers a rich playground to understand the basic physics and chemistry of magnetism in solids. To more easily share magnetic structural parameters between different computer programs, magnetic structure descriptors have been internationally stipulated and added to the Crystallographic Information File lexicon. The uniform description of magnetic structures is facilitating the formation of magnetic structural databases (e.g., MAGNDATA, Bilbao Crystallographic Server, https://www.cryst.ehu.es/) and the common format allows easy input for analysis and visualization programs. The database MAGNDATA now contains over 1,000 critically evaluated magnetic structures. Most magnetic struc-
tures have chemical and magnetic cells that are the same size and that have no structural changes accompanying the magnetic ordering. However, magnetic structures can be quite complex and go well beyond simple collinear ferromagnetic and antiferromagnetic arrangements. The magnetic cells can be large, even incommensurate, and contain complex noncollinear spin-spiral arrangements. Computational tools are freely available to solve and refine magnetic structures. The Bilbao Crystallographic Server (https://www.cryst.ehu.es/) and the ISOTROPY Software Suite (https://stokes.byu.edu/iso/isotropy.php) are indispensable. For full details, see references cited on those web pages.

Of geoscience relevance, a handful of (Fe, Mn, Ni)-bearing minerals magnetically order above room temperature and can contribute to rock magnetism. To understand this better, there are two types of relevant temperature: 1) the Néel temperature ($T_N$), which is the temperature limit at which an antiferromagnetic material becomes a paramagnet; 2) the Curie temperature ($T_C$), which is temperature above which a ferromagnetic material loses its magnetic properties. Examples of magnetically ordered minerals include hematite ($T_N \approx 680 \, ^\circ C$), trevorite ($T_C \approx 585 \, ^\circ C$), magnetite ($T_C \approx 578 \, ^\circ C$), maghemite ($T_C \approx 600 \, ^\circ C$), magneisoferrite ($T_C \approx 440 \, ^\circ C$), pyrrhotite ($T_C \approx 325 \, ^\circ C$), jacobsite ($T_C \approx 300 \, ^\circ C$), and greigite ($T_C > 300 \, ^\circ C$). In contrast, and for materials of interest to physicists, the magnetic structures of hundreds of mineral phases have been studied largely to understand magnetic ordering in a more expansive range of chemical structures and, more recently, to search for novel examples of so-termed “frustrated magnetism” (e.g., Inosov 2018). Most physicists have used synthetic analogs of minerals to ensure pure compositions. The minor element impurities
common in minerals often confound the magnetic ordering behavior, making actual minerals unsuitable samples from the materials physics perspective. Nevertheless, mineral structures inspire many magnetic structural studies of their synthetic analogs, and minerals are often studied themselves, particularly when large single crystals are available which are ideal for neutron diffraction.

A good and simple mineralogical example is the triphylite–lithiophilite solid solution Li(Fe,Mn)PO₄ which has the olivine structure and is technologically significant as a battery cathode. It has the light element Li and some transition metals on the same site that differ by one atomic number (Fe, Mn), and antiferromagnetism at low temperatures over the whole compositional range (lithiophilite LiMnPO₄ Tₘ = 34 K; triphylite LiFePO₄ Tₘ = 52 K). Although antiferromagnetism in triphylite–lithiophilite is not of particular interest geologically, large, relatively pure, single crystals (of centimeter size or more) covering the solid solution range can be found in granitic pegmatites making them ideal for single-crystal neutron diffraction. All of these attributes are why triphylite–lithiophilite has been featured as a single-crystal diffraction exercise at the National School on Neutron and X-ray Scattering for many years (pers comm. BC Chakoumakos and HB Cao). Symmetry analysis enumerates the possible range of magnetic structures, and these models can be tested against the measured diffraction patterns to identify which arrangement provides the best fit. The refined magnetic moment magnitudes (4–5 μₓ) fall in the expected range for many years (pers comm. BC Chakoumakos and HB Cao). Symmetry analysis enumerates the possible range for many years (pers comm. BC Chakoumakos and HB Cao). Symmetry analysis enumerates the possible range for many years (pers comm. BC Chakoumakos and HB Cao).

Figure S (A) Magnetic structure of α-Fe₂O₃ hematite above the Morin transition temperature. (B) Magnetic structure of α-Fe₂O₃ hematite below the Morin transition temperature. The Morin transition is a magnetic phase transition in α-Fe₂O₃ hematite for which antiferromagnetic ordering is reorganized from being aligned perpendicular to the c-axis above 262 K to being aligned parallel to the c-axis below 262 K, this temperature being known as the Morin temperature. In these cases, the magnetic space groups do not exhibit the highest symmetry possible. k = (0,0,0) conveys that the magnetic unit cell and the crystal structure unit cell are the same. Abbreviations: m = magnetic moment component for relevant x, y, z axis; μₓ = Bohr magneton. AFTER HILL ET AL. (2008).

Neutron diffraction provides great fidelity in determining the Mn/Fe composition, lithium site vacancies, atomic positions, and atomic displacement parameters.

Another example studied extensively is α-Fe₂O₃ (hematite). Hematite has the corundum-structure space group R̅3c and, below Tₘ ~ 955 K, the magnetic moments of Fe³⁺ adopt an antiferromagnetic structure aligned perpendicular to the c-axis. A further magnetic phase transition occurs at 262 K, the so-called Morin transition, where the antiferromagnetic ordering changes from perpendicular to parallel alignment with the c-axis. Shull et al. (1951) correctly deduced the magnetic structures of both of these phases by comparing the calculated with the observed magnetic peak intensities for various spin configurations. Magnetic space group analysis (Fig. S) shows that each magnetic moment component (mₓ, mᵧ, mₗ) can be variable within this spin arrangement. Nevertheless, above the Morin transition, only an mₓ component is refined by most diffraction measurements: a weak ferromagnetic component (~0.004 μₓ) along the [120] direction, perpendicular to the x direction, is realized but not explicitly shown. And a growing number of studies indicate a small out-of-plane component normal to the basal plane of the hexagonal axes (Brok et al. 2017 and references therein). For the low-temperature phase, the principal component lies along the c-axis with a smaller component along the a-axis.

Magnetism in hematite solid solutions gets more interesting due to some intergrowths of Fe–Ti oxides that can show high magnetic remanence and stability, greater than that of the individual phases. The lamellar magnetism hypothesis put forth to explain this is that such high and stable natural remanent magnetization is related to magnetic coupling across the interfaces between the phases, such as fine ilmenite exsolution lamellae in a host of titanohematite (Brok et al. 2017). Such effects are well-known in engineered multilayer heterostructures and are the basis...
for important technologies. It is evident that exsolution microstructures also play an important role in mineral magnetism and that they may be preserved in the lower crust. However, more experiments at relevant temperature and pressure conditions are needed. Here again, neutron diffraction and reflectometry are essential tools for these important studies.

Another example relevant to planetary science is the HP behavior of magnetic ordering in pyrrhotite (Fe₇S₈). Rochette et al. (2003) have shown that magnetic ordering in pyrrhotite is suppressed above 2.8 GPa, which has interesting implications for the origin of magnetic anomalies on Mars where pyrrhotite is believed to be one of the more significant magnetic minerals. We know from orbital magnetometer surveys that Martian crustal magnetic anomalies become demagnetized around impact craters, where pressure has exceeded ~3 GPa. If the crust is not remagnetized after impact, this implies that no Martian magnetic field existed at the time of the impact, and, thus, that these impact craters can be used to determine the timing of the shutdown of the Martian magnetic field.

Not all magnetic materials produce long-range ordered states. Some retain disorder with short-range magnetic correlations which manifest as diffuse scattering below, and above, their transition temperatures. Various examples of this frustrated magnetism are found in spin liquids, spin ices, spin glasses, multiferroics, and unconventional superconductors. A mineralogical example of a frustrated magnet is bixbyite, (Mn³⁺)₂O₃. Roth et al. (2018) used natural single crystals (also containing some Fe³⁺) from a rhyolite to measure the magnetic diffuse scattering and develop a model-free approach for direct reconstruction of magnetic correlations by 3-D difference pair distribution function analysis (Fig. 6). The neutron diffraction analysis and magnetic property measurements support that this bixbyite lacks long-range magnetic order and is a spin-glass below 32 K.

Consider again MnO. Previous neutron scattering studies have shown structured magnetic diffuse scattering is present above $T_N$ from short-range spin correlations persisting into the paramagnetic state. This is observed in the powder diffraction as a broad hump in the background that increases with decreasing temperature (Fig. 4B). Paddison et al. (2018) used reverse Monte Carlo analysis to fit single-crystal magnetic diffuse scattering in MnO and determine the local magnetic correlations, showcasing another model-independent alternative for interpreting diffuse scattering. Studies of magnetic (and nuclear) diffuse scattering ideally use single crystals to provide large and richly decorated reciprocal space volumes. However, when only powder samples are available, analysis of magnetic diffuse scattering can use the magnetic pair distribution function approach (Frandsen 2018), this being a new cousin to the highly successful total scattering pair distribution function method.

![Figure 6](image.png)

(A) Bixbyite—technically Mn³⁺₂O₃ but most commonly also with some Fe, giving (Mn³⁺,Fe³⁺)₂O₃—is cubic (Ia₃) and has two distinct metal sites (green and blue), both occupied by Fe and Mn. (B) The metal-only sites form a corner-sharing network of nearly ideal hexagons which manifest so-called frustrated antiferromagnetic interactions. (C) Single-crystal magnetic diffuse scattering is below 32 K; data collected using the Oak Ridge National Laboratory Spallation Neutron Source’s CORELLI diffractometer. (D) A special Fourier transform of the magnetic diffuse scattering for the metal-only sites allows the average spin-spin correlations to be visualized in real space. A negative peak indicates opposite alignment of spins (blue); a positive peak indicates parallel alignment of spins (red). After Roth et al. (2018).
SUMMARY
The unique scattering characteristics of the neutron have been successfully used to study nuclear and magnetic structural transitions: such studies started soon after high-intensity neutron beams became available at dedicated reactor sources. Modern neutron scattering technical developments have enabled the determination of precise in situ nuclear and magnetic phase transitions. Importantly, continuous and synergistic technical developments in both source and sample environments have been, and continue to be, key to experimental studies. New technical developments in both large volume and chemical vapor deposition diamond-based cells now push the limits to even lower- and higher-temperature studies at simultaneous high pressures.

ACKNOWLEDGMENTS
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REFERENCES
B y exploiting the penetration, attenuation, and scattering properties of neutrons, images of matter in two or three dimensions reveal information unobtainable using other probes. Despite the limitation in brilliance of neutron sources, several neutron-based imaging techniques are essential to different aspects of modern geoscience. Typical examples include the evaluation of porosity in rocks and sediments, mapping of light elements in solids, noninvasive probing of cultural heritage objects, investigations of thick engineering components, and the exploration of diffusion and percolation processes of fluids within porous matrices, organo-inorganic composites, and living organisms. Techniques under development include simultaneous neutron and X-ray tomography in heterogeneous media, Bragg-edge imaging, and the possibility of porosimetry from dark-field imaging.

Keywords: neutron imaging; radiography; tomography; microscopy; Bragg-edge imaging

INTRODUCTION

Neutrons can be used effectively in all areas of materials characterization, including imaging, crystallography (phase identification and quantification, strain and texture analysis, microstructural characterization), and chemical analysis (elemental and isotopic quantification).

Broadly speaking, scientific imaging extracts spatially resolved information from a given sample. We commonly think about direct imaging, such as making observations through a light microscope, where the experiment straightforwardly offers a detailed two-dimensional (2-D) view of the object in reflection or transmission. Neutron-based (and X-ray–based) probes use a beam of particles that can penetrate through a sample, meaning that the transmission imaging process is one based on the characteristic interaction between the probe and the material. The parameter most commonly measured by X-ray and neutron radiography is the absorption contrast, which is then converted to grey-tone or fake-color visual contrast in the image. However, the different cross-sections of elements with X-rays (electron interaction) and neutrons (nuclear interaction) makes the two probes perfectly complementary in the investigation of matter, and neutrons can be efficiently exploited to enhance sensitivity of the imaging experiment to light atoms or even specific isotopes. Three-dimensional (3-D) tomographic images can be formed from raw 2-D images using computational algorithms, such as the filtered back projection for which G. N. Hounsfield and A. M. Cormack received the Nobel Prize for Physiology or Medicine in 1979. Both neutron radiography and tomography have long been used to probe geological materials (e.g., Figs. 1 and 2) (Carlson 2006; Winkler 2006).

Beyond transmission mode, there are several more complex techniques that can yield indirect views of matter distribution within a solid: these are based on the different ways one can analyze the neutrons that are scattered by a sample (Anderson et al. 2009; Brenizer 2013). Neutron activation autoradiography involves measuring the decay time of the activated species from neutron-induced gamma activation to produce a chemically resolved map, which may be roughly considered as the neutron equivalent of a chemical map produced by X-ray fluorescence spectroscopy. Other more complex techniques are based on scattering- or diffraction-enhanced imaging (Woracek et al. 2018; Tran et al. 2021) and will be briefly described herein.

Because neutron sources are weak compared to photon and electron sources, it necessarily shifts the experimental requirements towards larger beams and larger sample volumes. In many cases, the use of large samples is advantageous, e.g., to capture representative volume elements in porous media, map the internal features of fossil organisms, or investigate other sample types such as cultural heritage objects (e.g., paintings and statues). However, needing both a large beam and a large object volume severely limits the spatial resolution commonly accessible in neutron imaging. State-of-the-art neutron imaging techniques are striving to reach voxel (“3-D pixel”) resolutions in the micrometer range, compared to the nanometer resolution achievable with photon and electron beams.

Before sampling at submicrometer resolution and tackling the problem at molecular and atomic resolution, it is important to assess the representative nature and integrity of the sample volume to be investigated. Neutron imaging is, thus, a flexible and penetrating tool to investigate the inner features of a geological sample at the macro- to micrometer-scale. These features can include, but are not limited to, fossils (Dawson et al. 2014), biominalized specimens (Fig. 2), meteorites (Fig. 1) (Fedrigo et al. 2018), oil-hosted reservoir rocks (Chiang et al. 2018), and porous sediments (Cordonnier et al. 2019). The 3-D visualization...
and quantification of inner surfaces and interfaces between components are the key to interpreting and modeling those components.

Our goal here is to describe how neutron imaging contributes to the geosciences and to cultural heritage by focusing on the following: (1) fluid–rock interaction and the quantitative assessment of the pore systems in geological materials; (2) the diagnostic use of neutrons to characterize cultural heritage materials and objects. Because of the complexities in accessing and using neutron-source facilities, besides the analysis and interpretation of the imaging data, it is suggested that synergies between Earth scientists and cultural heritage researchers, who traditionally lack experience as neutron users, be substantially enhanced and expanded to benefit the field.

### Figures

**Figure 1** (A) Photograph of the Monturaqui impactite sample (Chile). (B) The segmented image of a section of the sample deduced by combined X-ray and neutron tomographic information. (C) Vesicles distribution in the impactite. FROM FEDRIGO ET AL. (2018).

**Figure 2** Images from neutron investigations of cultured pearls. (A) Neutron data provide a remarkable contrast between the organically enriched layers (lighter), the aragonite-based biomineralized matrix (darker), and the hollow core (irregular surface). Data collected at the IMAT beamline (at the ISIS Neutron and Muon Source at the Rutherford Appleton Laboratory, UK). Voxel size 55 μm. See also TABLE 1. FROM VITUCCI ET AL. (2018). (B and C) X-ray microtomographic images of two cultivated pearls. The cultivation seed and its interface with the naturally grown layer can be directly imaged, albeit with limited contrast between the carbonate/organic core and the aragonitic overgrowth. Images taken using the Laboratory Bruker-Skyscan 1172 instrument; voxel size 4.5 μm. IMAGES COURTESY OF L. VALENTINI, UNIPD.

### INSTRUMENT DEVELOPMENT AND TRENDS

Neutron imaging has developed rapidly over the past two decades and is now an essential component of user programs at national neutron sources. Beamlines devoted specifically for imaging are now among the first to begin operating at the two newest planned neutron sources of ESS and RA-10 (see Table 1). This development is due to improvements in neutron image spatial resolution; improvements in the use of multimodal imaging methods that can facilitate volume segmentation (i.e., identification, labeling, and separation of the voxel of interest, often visualized as separated images); and improvements in image contrast due to polarization, diffraction, and refraction. We provide an overview on these methods (except for polarization) in the following section.

#### Simultaneous Neutron and X-Ray Imaging

The technique of simultaneous neutron and X-ray tomography (NeXT) takes advantage of the complementary nature of the two modalities to readily identify material phases within a heterogeneous sample. This is particularly advantageous when in the presence of highly contrasting materials, such as porous media that typically contain a hydrogenous material (e.g., water) within a mineral matrix (e.g., a porous carbonate or silicate rock): X-rays have good sensitivity for the matrix, while neutrons have good sensitivity for the hydrogen-containing fluids.

Although simultaneous acquisition is not essential for static cultural heritage specimens, it is critical to capture stochastic, time-evolving phenomena such as fluid flow in soils or geological matrices and the evolution of concrete degradation or repair. To make the NeXT technique work, one must remove crosstalk between the two sources, so that the neutron camera only detects neutrons, and the X-ray camera only detects X-rays. LaManna et al. (2017) oriented the X-ray tube orthogonal to the neutron beam and shielded the neutron detector with a thin (~5 mm) sheet of lead, while the X-ray detector was shielded with a thin (~2 mm) sheet of lithiated plastic. The time resolution of NeXT is dominated by the intensity of the neutron beam, which is of order 10⁶ cm⁻² s⁻¹. To obtain a reasonable tomographic reconstruction with conventional algorithms from this intensity requires an acquisition time ~1 day for a voxel size ~10 μm. By sacrificing spatial resolution (having a minimum of 200 μm) and reduced angular sampling (155 projections vs. ~1,000), one can reduce the data acquisition time to ~1 s (Tőtzke et al. 2019). The quality of the reconstructions can be further improved by using iterative algorithms based on knowledge of a prior state (Vitucci et al. 2018) or using emerging machine learning algorithms.

The utility of NeXT data is apparent during the task of segmentation, where one attempts to define a region of a given composition (Chiang et al. 2018). One computes a bivariate histogram after ensuring that the two reconstructed volumes are digitally registered, and many software
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platforms now have built-in functions to perform these tasks. By selecting regions of interest using the bivariate histogram, one can obtain robust segmentation of different material phases. The segmentation can be improved by additional smoothing, for instance by applying a nonlocal means filter.

**Neutron Microscopy**

Neutron microscopy involves imaging at a spatial resolution better than 10 μm. There are basically two types of neutron sources: continuous, and pulsed. A pulsed source is the more challenging in terms of reaching high spatial resolutions. The advantage of the pulsed source is that by tagging the arrival time of the neutron after the generation of the pulse, one knows the wavelength (or energy) of the neutron, which is important for the emerging methods discussed below. Pulses are generated at a frequency of 10–60 Hz, so to have an adequate wavelength resolution requires tagging the neutron arrival to a 10–100 μs precision. The time-averaged event rate over an area of 10 cm² is up to 10⁶ s⁻¹. Thus, the readout electronics for a pulsed source neutron imaging detector must be very fast to record each individual event at an event rate of about 10 GHz. The latest generation of Medipix chips coupled with neutron-sensitive microchannel plates (Siegmund et al. 2007) promise to meet three requirements: 1) single-event times better than 100 μs; 2) spatial resolution at least 10 μm; 3) a global event rate of 10 GHz. However, despite the time resolution of the detector and because of the neutron intensity, it will still take many tens of minutes to achieve good counting statistics. This is also a limitation for continuous neutron sources.

For continuous neutron sources, one does not need to resolve individual neutron capture events, which greatly simplifies detector requirements. The most common neutron imaging detector setup is a very-low-noise digital camera that can view a neutron-sensitive scintillator. The rapid advance of digital cameras with very low noise, very high detection efficiency, and pixel pitch on the order of 5 μm, means that the spatial resolution in this configuration is primarily limited by the “light bloom” in the scintillator. When the neutron is captured, energetic charged particles deposit energy to the scintillator, which is then released as visible light. Both the range of the charged particles and the amount of scattering of the light (which scales with the thickness) influence the size of the light bloom. Gadolinium is a good neutron scintillator material because it has a very large neutron absorption cross section so that very thin scintillators can be made while maintaining high neutron detection efficiency. In fact, by creating scintillators from isotopically enriched 157Gd, one can have almost 100% neutron absorption in a scintillator just a few microns thick (Trtik et al. 2015). The range of the conversion electrons that result from the neutron capture is similarly limited to a few micrometers.

**Wavelength-Selective Neutron Imaging for Multiscale Images**

High spatial resolution and fast temporal resolution require one to average over the full polychromatic spectrum of the neutron beam. If one relaxes the spatial and/or temporal resolution requirements, it is possible to form images at different wavelengths, enabling sample sources of image contrast to be revealed that would otherwise be well below the best direct spatial resolution. In the following two subsections, we introduce two such techniques: Bragg-edge imaging, and dark-field imaging.

**Bragg-Edge Imaging**

From Bragg’s law of diffraction, \( n \lambda = 2d \sin \theta \), we see that if \( \lambda > 2d \), then \( \theta \) is undefined and the lattice plane, \( d \), having Miller indices \( hkl \), no longer contributes to scattering. The transmission as a function of \( \lambda \) will show an increase (i.e., Bragg-edge) that is proportional to \( \lambda^2 \) and the structure factor. The scattering direction at the Bragg-edge is along the beam propagation axis, but in the backward direction. The typical wavelength range of neutron imaging instruments is 0.1 nm to 10 nm, and this means that the unit cell of many crystal structures can be observed, so enabling one to probe the strain along the beam direction, to understand the distribution of texture, and to

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**Table 1**

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**Notes:**

1. Full institute names are as follows: NIST = National Institute of Standards and Technology (USA); ORNL = Oak Ridge National Laboratory (USA); CNEA = Comisión Nacional de Energía Atómica (Argentina); ANSTO = Australian Nuclear Science and Technology Office; J-PARC = Japan Proton Accelerator Research Complex; CSNS = Chinese Spallation Neutron Source; FLNP = Frank Laboratory of Neutron Physics (Russia); ESS = European Spallation Source (Sweden); MLZ = Max–Planck Gesellschaft (Germany); PSI = Paul Scherrer Institut (Switzerland); ILL = Institute Laue–Langevin (France); ISIS = ISIS Neutron and Muon Source (UK).

2. Availability for user operation. If not in operation a start date is provided.

3. Spectrum types include the following: constant wave thermal (CWT), constant wave cold (CWC), pulsed thermal (PT), and pulsed cold (PC), where a thermal neutron spectrum has characteristic wavelength of 0.2 nm or less and a cold spectrum has characteristic wavelength larger than 0.2 nm.

4. Institute offers (or plans) simultaneous neutron and X-ray tomography.

5. Institute offers (or plans) neutron grating interferometry.

6. Institute offers (or plans) Bragg-edge imaging.
measure crystal phase fractions. The appeal of Bragg-edge imaging is higher spatial resolution (50 µm) maps of the crystallographic details than is possible with conventional neutron strain scanners, which have a gauge volume (i.e., a sampled volume) on the order of 1 mm$^3$. Modeling the coherent elastic scattering cross section for Bragg scattering (Woracek et al. 2018) can yield the strength of the texture, the preferred crystal orientation, and the crystallite size.

Bragg-edge imaging of crystalline materials can be successfully conducted using either pulsed or continuous sources (Vitucci et al. 2018). If one is analyzing strain in only one lattice plane or the phase fraction of two phases, using a monochromator at a continuous source is efficient because only a narrow wavelength bandwidth is required. Woracek et al. (2018) used this property when they performed tomography measurements of the volume fractions of austenite and martensite in transformation-induced plasticity steels subjected to torsion.

DARK-FIELD IMAGING

Neutron dark-field imaging is an emerging method that produces images of a sample’s microstructure that are well below those available from direct spatial resolution. Dark-field images are formed by looking at the change in the amplitude (or visibility) of a Moiré pattern (a beam that has a sinusoidally varying intensity in one direction). A detailed analysis by Wen et al. (2008) showed that this change is due to small-angle neutron scattering from the sample, and this can provide information about inhomogeneities at the microscale in each pixel of the image. The appeal of dark-field imaging for the geosciences is that it enables one to capture 3-D pore structure at the nanometer to micrometer scales, which is orders of magnitude less than by using conventional core sample sizes (diameters on the centimeter scale). Obtaining this 3-D multiscale data set involved acquisition and analysis process. The multiscale being measured is set by the period of the Moiré pattern, the wavelength of the beam, and the distance between the sample and the detector. For tomography, one acquires Moiré images as the sample is rotated 360°. One uses conventional tomography reconstruction algorithms to form two images, the usual transmission image (average of the Moiré pattern), and dark-field image (amplitude of the Moiré pattern). By acquiring these tomograms at varying multiscales one can, for instance, map out the pore distribution in each voxel (Harti et al. 2018). Whereas small-angle neutron scattering requires thin samples to avoid multiple scattering, and averages over a diameter of about 1 cm, dark-field imaging measures similar microscale quantities but in thick samples and with voxel size of ~50 µm. An example of the final output of such a measurement is shown in Figure 3. This assumed that the granite sample used was entirely quartz (a good approximation for the rock matrix) scattering length density) and so estimated three important parameters: pore size, volume, and distribution.

The imaging requires detailed 3-D analysis in order to interpret the properties of the samples, their evolutionary mechanisms, and/or any rate of change.

The investigation of porous media is particularly suitable to neutron imaging (e.g., Cole et al. 2009) because of the natural contrast between pore fluids (air, water, hydrocarbons) and contact minerals or rock matrix. In fact, percolating fluids such as water and oil are hydrogen-rich, and hydrogen strongly attenuates a neutron beam due to its large incoherent scattering cross section, making visible any fluids present in an inorganic, variably saturated medium (Perfect et al. 2014). The applications span from the simple evaluation of pore volume in consolidated rocks or loose soil, to the measurement of water flow through a pore system and the quantitative assessment of media permeability using dynamic neutron transmission radiography (Fig. 4) (e.g., Cnudde et al 2008, Zambrano et al. 2019). The information gained through imaging experiments are important for the interpretation and prediction of all processes born out of fluid–rock interactions: for example, the management of water resources, the recovery of hydrocarbons, the diffusion and migration of pollutants through sediments, the rheology of saturated geomaterials during landslides, or the durability and stability of waste repositories. The processes involving multiscale mechanisms and the prediction of fluid flows in media having multiscale

APPLICATIONS TO EARTH AND PLANETARY MATERIALS

Earth and planetary materials are naturally heterogeneous and complex. Neutron imaging investigations greatly help in elucidating such complex features as rock textures, mineral boundaries, the surfaces of mineral assemblages, and the behavior of fluids in confined pores and fractures.
porous systems benefit greatly from quantitative neutron imaging experiments. In the case of highly saturated materials, the quantitative assessment of the pore fluid may need an appropriate correction to the recorded images. Furthermore, air trapped in macro pores may substantially change the permeability models of the media (Snehota et al. 2015), and, in this case, combined neutron and X-ray tomography experiments allow appropriate assessment of the two-phase flow mechanism through the pore system (Kaestner et al. 2016). Recent experiments based on combined neutron and X-ray tomography modalities, such as the NeXT arrangement described above, allow one to characterize the dynamics of water absorption in a claystone by comparing material deformation as well as water arrival (Stavropoulou et al. 2020).

The mechanical behavior of porous rocks and their effect on fluid flow is particularly important in hydrocarbon production and CO2 sequestration. The measurement of localized strain through imaging techniques (Tudisco et al. 2015) or the direct measurement of strain partitioning by diffraction methods provide experimental background to model the response of geological materials to external forces and understand how the deformation caused by force gradients is accommodated within the sample.

THE POTENTIAL OF NEUTRON IMAGING IN CULTURAL HERITAGE DIAGNOSTICS

Despite the large number of neutron techniques available, the single most used technique for the characterization of cultural heritage materials and objects is neutron activation analysis, which employs a neutron beam to irradiate the sample and activate all possible nuclear decays within the material. The use of neutron activation analysis dates to the early days of dedicated neutron sources, and it has been especially applied to the chemical analysis of ancient ceramics, glass, and stone artifacts. These analyses still stand as a reference for modern research, providing a complementary framework for probing natural and experimental geological materials.

Of course, neutron radiography has also been very popular, because of the ease of inserting large objects into penetrating neutron beams and obtaining real-size images of the objects’ interior. A very specific technique, one widely used in conservation and art history of paintings, is the combination of radiography and neutron activation, called neutron activation autoradiography. It is based on the activation of secondary emission processes within the painting by the neutron irradiation of the whole object and by detecting the γ-emissions at different times in the form of 2-D images (the autoradiography part) (e.g., Kardjilov and Festa 2017). The technique was very popular for the systematic analysis of museum paintings, but it will be limited in the future by the lack of open ports at reactor sources.

Beyond autoradiography, a number of techniques developed in recent years for materials science and crystallography have also been applied to cultural heritage problems and materials (Kardjilov and Festa 2017). The two areas most rapidly increasing in quality and range of applications are neutron tomography and neutron crystallography. Neutron tomography is the production of 3-D images from the detection of absorbed neutrons in the sample; in a sense, it is a natural development of neutron radiography. The characteristics of neutron beams make modern neutron tomography an invaluable tool for art and archaeological research, especially for the preliminary analysis of art objects before and during the planning of conservation strategies. Archaeological and artistic metals are great candidates for neutron imaging investigations (e.g., Salvemini and Grazzi 2017) because neutrons nicely probe below the surface and allow a clear vision of the inner features, which would be hard or impossible to map by X-rays. Typical applications include the ability to detect organic compounds (flowers, glue, resins, textile, paper) embedded in metal objects. Previous conservation treatments of museum objects, often unrecorded, may be easily spotted using neutron imaging, especially if they were carried out by organic consolidants or preservatives.

It is expected that integrated research (i.e., research that couples imaging, diffraction, and spectroscopy) will be possible due to the increased neutron flux and energy resolution of the sources now coming on stream. This will provide a far greater density of complementary information and, at the same time, limit the neutron dose absorbed by art and museum objects and the subsequently induced radioactivity imparted to the object. Recent combined experiments that coupled imaging and diffraction, or imaging and prompt gamma activation analysis (e.g., Kardjilov and Festa 2017), are leading the trend. Neutron resonance transmission imaging is also a sensitive analytical technique useful for performing both qualitative and potentially quantitative multi-element analysis of major, minor, and even trace elements, providing 2-D maps of element abundance in a variety of materials (Fedrigo et al. 2019).

As described above, Bragg-edge imaging (Woracek et al. 2018), also called spectral neutron imaging (Tran et al. 2021), is efficiently using diffraction information collected in a spatially resolved mode. The possibility of extracting crystallographic information from the data measured at different energies, and thereby discriminating between different phases in reconstructed 3-D images, is a great advancement in the interpretation of manufacturing
processes and of various types of degradation process. The well-investigated case of Japanese katana blades (Fig. 5) (Salvemini and Grazzi 2017) revealed the complex manufacturing process, which involved a controlled martensitic transition in just a part of the blade, and is a good example of the great potential of diffraction-enhanced imaging.

Neutron imaging and neutron characterization methods in general are extremely useful in cultural heritage investigations, although neutron instruments are only being extensively used when there are strong collaborations with beamline scientists. A more extensive implementation of coordinated effort, and with focused infrastructures, may possibly help in knowledge diffusion and, ultimately, a better use of the existing and developing facilities.

FUTURE OUTLOOK

As the methods of Bragg-edge and dark-field imaging mature, it is expected that there will be more applications in the geoscience and cultural heritage fields to take advantage of structural characterization studies. New pulsed neutron imaging sources will soon be commissioned (see Table 1) that will make these methods routine by exploiting the time structure of the beams. In terms of neutron microscopy, creating an analog of Hooke’s microscope by using reflection-based neutron lenses (so-called Wolter optics) has the potential to dramatically improve the time resolution while concurrently maintaining high spatial resolution (5 µm), even in the presence of bulky sample environments. Although not an application in the geosciences, the work of Jorba et al. (2019) showed that a prototype Wolter optic improved the resolution 5-fold while also increasing the time resolution by two while imaging the ferromagnetic transition of a quantum magnet that was in a cryostat (~90 K) and inside a pressure cell at 15 kbar. The design by Hussey et al. (2021) promises to obtain a spatial resolution of 3 µm with an exposure time of about 1 s, which, when combined with the ability to maintain spatial resolution even with bulky sample environments, will marry synchrotron-like image resolution with the penetrating power of neutrons. The Wolter optic microscope will likely be a powerful tool for many applications in the geosciences.

REFERENCES


ElEmEnts June 2021
**The Fourth Polymorph of Mg₂SiO₄: Poirierite in Shocked Meteorites**

Mineral physicists, using high-temperature and high-pressure experiments, have been trying to clarify the structural changes and phase equilibrium of minerals inferred to exist in Earth's deep interior. A variety of high-pressure phases of silicates and oxides have now been synthesized. In nature, such phases have been found mainly in shocked materials from terrestrial impact craters and stony meteorites, because high-velocity collisions effectively simulate the high-pressure and high-temperature conditions in Earth's deep mantle. Mineralogists have been enthusiastically using transmission electron microscopy (TEM) to hunt down high-pressure minerals after the discoveries of MgSiO₃-ilmenite (akimotoite) and MgSiO₃-perovskite (bridgmanite) in shocked chondritic meteorites during the late 1990s (Sharp et al. 1997; Tomioka and Fujino 1997, 1999). Currently, over 30 high-pressure minerals have been discovered in natural rocks.

Olivine [(Mg,Fe)₂SiO₄] is the most common constituent mineral in the Earth's upper mantle. It transforms into a spinellloid structure (wadsleyite) and a spinel structure (ringwoodite) with increasing pressure. These high-pressure minerals are considered dominant in the mantle transition zone at depths of 410–660 km. Meteoritic wadsleyite and ringwoodite often show nanometre-scale planar defects observable only under a TEM. Based on the observations of the defect structures, combined with the topological analyses of the crystal structures of the olivine polymorphs, shear mechanisms without long-range ionic diffusion are posited to promote polymorphic transformations. The transformation model also predicts the possible occurrence of an intermediate spinellloid structure (ε phase) (Madon and Poirier 1983). This hypothetical phase remained undiscovered in high-pressure synthesizes products and natural samples for more than three decades. Our high-resolution TEM studies, however, have recently clarified that the ε phase is present in shocked chondrites (Tomioka et al. 2021). The phase has been approved as a new mineral species by the International Mineralogical Association's Commission on New Minerals, Nomenclature and Classification and named “poirierite” in honour of Jean-Paul Poirier, who greatly contributed to mineral physics, including the theoretical prediction of ε-Mg₂SiO₄.

In the Miami and Tenham chondrites, wadsleyite and ringwoodite occur as monomineralic aggregates entrapped in shock-induced melt veins. These occurrences suggest that the olivine grains in the host rock were initially transformed into stable high-pressure phases by nucleation and growth mechanisms in prograde shock metamorphism without melting. The nanoscale lamellar poirierite is topotactically intergrown within the wadsleyite and ringwoodite grains (Fig. 1). Single-crystal X-ray diffraction analysis of poirierite coexisting with ringwoodite in the Suizhou chondrite, as well as the results from first-principles calculations, confirmed that poirierite has an orthorhombic unit cell having the smallest dimensions of any of the pre-existing spinellloid structures (Fig. 1). Rapid cooling and decompression during retrograde shock metamorphism would have hindered the direct back-transformations from wadsleyite/ringwoodite to olivine but would have promoted the metastable formation of poirierite by a shear mechanism.

The formation processes of high-pressure minerals, including poirierite, are closely related to the pressure–temperature–time histories of impact events. The pressure values deduced from phase equilibria of meteoritic components provide mutual collision velocities of their parent bodies. Shock pressure durations, estimated from phase transformation kinetics and element diffusion in meteoritic high-pressure minerals, provide the sizes of impactors. The mineral formation process when combined with the radiometric ages of shock events of meteorites provides more robust constraints for the theoretical models of the evolution of the early Solar System. Such knowledge also potentially contributes to a better understanding of the dynamics of the deep Earth.

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**JOURNAL OF MINERALOGICAL AND PETROLOGICAL SCIENCES**

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**Original Articles**

Evolution of supracrustal rocks of the Indochina Block: Evidence from new detrital zircon U–Pb ages of the Kontum Massif, Central Vietnam — Kenta KAWAGUCHI, Pham MINH, Pham Trung HIEU, Truong Chi CUONG, Kaushik DAS

Anatomy of Shaku–dake high–Mg diorite, southwest Japan: Lithofacies variations and growth process of high–Mg diorite stock — Keisuke ESHIMA

Crystal structure of nesquehonite, MgCO₃·3H₂O by neutron diffraction and effect of pH on structural formulas of nesquehonite — Gen-ichiro YAMAMOTO, Atsushi KYONO, Jun ABE, Asami SANO-FURUKAWA, Takanori HATTORI

**Letters**

Zairite in quartz veins from Ishidera area, Wazuka, Kyoto Prefecture, Japan — Yuma MORIMITSU, Yohei SHIROSE, Satomi ENJU, Kenji TSURUTA, Norimasa SHIMOBAYASHI

Trace and rare earth element geochemistry of clinopyroxene in mafic dykes from Western Dharwar craton, southern India — Sasidharan A. SILPA, M. SATISH–KUMAR, Eiichi TAKAZAWA, Krishnan SAJEEV
The International Association of GeoChemistry (IAGC) is happy to announce the recipients of the 2021 Student Research Grants, sponsored by Elsevier and the IAGC. This is a very competitive award, with a funding rate of around 10% in 2021. The success of these grantees demonstrates the extremely high caliber of their research. Congratulations to all our grantees! Next year’s applications will be accepted starting in October 2021 – check our website for details or follow us on Twitter at @IAGeoChemistry.

**Andrea Johansen** is a PhD candidate at the University of Wollongong (Australia) and a Residential Scholar at the Australian Institute of Nuclear Science and Engineering. She investigates atmospheric dust transport to islands in the South Pacific and Southern Oceans and the role of dust fertilization in peat primary productivity. Andrea uses a combination of trace element analysis and isotopic characterization (e.g., Nd and Pb isotopes) to reconstruct dust deposition records within peat mires, allowing dust to be provenanced to its source areas and so revealing how dust sources have switched on and off in response to climate variability. The peat cores are dated using 210Pb (by alpha spectrometry), the fallout radionuclides 239+240 Pu, and 14C (by accelerator mass spectrometry). Relative decomposition, which is needed to establish the primary productivity profile, is characterized by isotope ratio mass spectrometry of δ13C, δ15N, and CN96, along with Fourier transform infrared analysis of the organic carbon components. Andrea believes that a better understanding of dust transport and air-mass movements during the Holocene will improve our knowledge of the carbon storage function of the South Pacific and Southern Oceans.

**Madison Wood** graduated in 2019 with a BSc in Earth sciences, focusing on climate, from the University of New Hampshire (USA). She is now a PhD student at the University of California Santa Cruz (USA) in the Department Earth and Planetary Sciences, where she uses geochemical signatures of seawater chemistry preserved in marine sediments to reconstruct past changes in the carbon cycle. Her dissertation is on stable and radiogenic Sr isotopes in marine barite by thermal ionization mass spectrometry to reconstruct the Sr isotopic composition of the ocean over the past 500,000 years.

**Rebekah Rhodes** earned her BSc in geology from the University of North Carolina at Chapel Hill (USA) in 2012 and her MSc in geology from the University of Wyoming (USA) in 2015. After teaching high school science for two years, Rebekah began a PhD in 2017 at North Carolina State University (USA) concentrating on paleoclimate and geochemistry. Rebekah’s current research focuses on understanding how terrestrial climate varies spatially and temporally. More specifically, she is investigating the variability and sensitivity of climate during the Early Eocene Climatic Optimum (EECO) in southwestern Wyoming. Rebekah uses stable C, O, Sr, and clumped isotope analyses on carbonates from the Green River Formation as proxies for climate during the EECO. Additionally, Rebekah hopes to expand the applications of clumped isotope thermometry by testing the method on new materials. Rebekah believes that understanding how terrestrial climate responded to past warm periods will be vital in predicting how climate will be affected by future warming.

**Kristina Sukhanova** graduated in 2015 with a specialist (equivalent to a master’s) degree cum laude in mineralogy and geochemistry from the Mining University (St. Petersburg, Russia). She is currently a PhD student at the Institute of Precambrian Geology and Geochronology, Russian Academy of Sciences. Kristina is studying rare earth element (REE) mobility in silicate minerals from different types of ordinary chondrite (OC) meteorites. She uses a secondary ion mass spectrometer to measure concentrations of trace elements and REEs in olivine and pyroxene and to determine the U–Pb age of Ca-phosphate minerals. Studies of trace element composition in silicate minerals of unequilibrated OCs will help evaluate element mobilization under secondary processes (such as thermal and impact metamorphism, or fluid activity) on OC meteorite parent bodies. Her research will use, for the first time, trace element analyses on silicate minerals from equilibrated OCs. These data will describe the intensity of secondary processes and clarify the structure models of chondrite parent bodies. These data should also help in the petrological analysis of silicate materials from the Ryugu and Bennu asteroids.

**Vincent Clementi** earned his BSc in environmental science and policy from the University of Maryland (USA) in 2013. He is currently conducting PhD research in oceanography at Rutgers University (New Jersey, USA). Vincent’s dissertation focuses on pore-fluid origins, migration, and carbon cycling in the waters off the Chilean margin using new 100-meter-long sediment cores recovered during the 2019 JOIDES Resolution 100 expedition, which documented widespread freshening in pore fluids. With support from the IAGC, he is using the isotopes of O, H, and Sr in pore fluids to test the hypothesis that observed freshening and elevated dissolved silica concentrations at a site proximal to Northern Patagonia are driven by submarine groundwater discharge, which could have implications for the regional marine geochemical budget.
LETTER FROM THE PRESIDENT

The Spanish Mineralogical Society (SEM) elections took place at the last General Assembly, which was held October 2020 as an on-line event. We elected a new secretary, a new vice-secretary, and five councillors, all of whom will serve a four-year term on the executive council. The new council members are as follows (all institutions are in Spain): Nuria Sanchez Pastor (University Complutense of Madrid, secretary); Didac Navarro Ciurana (University of Barcelona and Autonomous University of Barcelona, vice-secretary); and councillors Cinta Barba Brioso (University of Seville); Jose María González Jiménez (University of Granada); Juan Morales Sanchez-Migallón (University of Salamanca); Rafael Pérez López (University of Huelva); and Encarnación Ruiz Agudo (University of Granada). On behalf of our members, I would like to thank all the outgoing councillors who served the society with such great efficiency and enthusiasm.

Top: (Left to right): Blanca Bauluz Lázaro (University of Zaragoza, SEM President), Nuria Sanchez Pastor (University Complutense of Madrid, secretary), Didac Navarro Ciurana (University of Barcelona and Autonomous University of Barcelona, vice-secretary). Bottom: (Left to right): councillors Cinta Barba Brioso (University of Seville), Jose María González Jiménez (University of Granada), Juan Morales Sanchez-Migallón (University of Salamanca), Rafael Pérez López (University of Huelva), and Encarnación Ruiz Agudo (University of Granada)

The SEM was created in 1975 by a group of crystallography and mineralogists scientists. The society has a long tradition of supporting initiatives that promote knowledge in the fields of mineralogy, petrology, geochemistry, and related sciences, as well as training teachers and researchers in these disciplines. Today, the society is in good shape, with a stable number of members at around 300. Moreover, the number of student members is increasing year after year. The SEM must remain young and dynamic. We have begun planning for the future and would like to focus our efforts on three core issues: 1) to increase international collaboration between academics and industry, and to increase collaboration among our own society members; 2) to improve SEM’s response to the needs of young mineralogists; and 3) to make society at large more aware of the importance of mineralogy. Every year the SEM announces grants to promote the dissemination of mineralogy, petrology, and geochemistry in primary and secondary schools and in wider society. We also give awards to MSc projects and to presentations by young researchers at conferences to show that we value their investigations.

Blanca Bauluz
SEM President

THE 2nd YOUNG RESEARCHERS CONFERENCE OF THE SPANISH MINERALOGICAL SOCIETY (SEM)

Organized by the Universitat Autònoma de Barcelona (UAB) and the SEM-CAT students association, the 2nd Young Researchers Conference of the Spanish Mineralogical Society (SEM) was held 22–24 March 2021 as an on-line event. The main objective was to hold student scientific sessions that would become platforms for debate and a means for exchanging ideas. The program included three sessions: 1) Mineral Resources; 2) Heritage, Environment and Water–Rock Interaction; 3) Crystal Growth, Mineralogy and Petrology. The abstracts can be downloaded from the SEM website (http://www.semineral.es/websem/).

Oral Presentations

In all, nearly 160 scientists were involved in 30 oral presentations, which were conducted by undergraduate, MSc, and PhD students from Spanish universities and research institutions. Contributions included topics on experimental mineralogy, descriptive petrology, interpretation of geochemical data, new mineral deposits, conservation of historical heritage, water and soil contamination, geochemical numerical simulations, synthesis and crystal growth, and the significance of clay minerals.

The program also included three invited lectures: “Mineralogy, Composition and Formation Mechanisms of Ni-Phyllosilicates in Nickelineiferous Laterites (Ni-Serpentine and Garnierites): EMP, MET and Raman Spectroscopy” given by Cristina Villanova de Benavent (University of Barcelona, Spain); “Mining Waste: A Potential Ceramic Resource” given by Francisco Veiga Simão (University of Leuven, Belgium); and “The Potential of Thin Sections in the Microstructural Studies of Ceramic Glazes” given by Roberta Di Febo (Autonomous University of Barcelona, Spain). All these scientific contributions have been published in volume 25 of *Macla*, which is edited by the SEM.

Awards for Young Researchers

Three awards were given to the best oral presentations of the conference. The winners were as follows: 1) Marta Henrich Grínó and Aleix Saiz Alexandre (Autonomous University of Barcelona, Spain) for their talk “Characterization and Genesis of the Balcoll Mineralization (Priorat, Catalunya): Outreach Proposal”; 2) Claudia Prieto Torrell (University of Barcelona) for her talk “Ankaramitic Lavas from El Hierro Island: Insights from Petrography”; 3) Elisa Laita (University of Zaragoza) for her talk “Mineral and Textural Transformations during Firing of Bauxitic Materials and their Relationship with Interesting Physical Properties”.

The organizing committee would like to thank all participants for this fruitful and excellent meeting. We are already looking forward to the 3rd European Mineralogical Conference (emc2022), which was postponed in 2020 due to the global situation with the coronavirus (COVID-19). The newly proposed date is 29 August–2 September 2021.

Didac Navarro Ciurana and Mercé Corbella
Organizing and Scientific Committee (Autonomous University of Barcelona)
MAC 2021 AWARDS

The Mineralogical Association of Canada (MAC) is pleased to announce its award winners for 2021

Peacock Medal to Dr. Thomas Stachel

The Peacock Medal is awarded to a scientist who has made outstanding contributions to the mineral sciences in Canada. There are no restrictions regarding nationality or residency. The medal is intended to recognize the breadth and universality of the scientist’s contribution to mineralogy, applied mineralogy, petrology, crystallography, geochemistry, or the study of mineral deposits, rather than in a narrow area of expertise. The Peacock Medal is the highest award bestowed by the Mineralogical Association of Canada (MAC) and is named in honour of late Professor Martin A. Peacock (1898–1950), a professor of mineralogy at the University of Toronto from 1937 until his untimely death in 1950.

This year’s awardee is Dr Thomas Stachel, a professor in the Department of Earth and Atmospheric Sciences at the University of Alberta (Canada) whose main research area is diamond geology.

Thomas was born and educated in Germany. Studying geology at Gutenberg University in Mainz (Germany), he became very interested in volcanology, and for his MSc thesis he worked with Georg Büchel on a geophysical investigation of the (then-termed) Tertiary maar diatremes in the Eifel Volcanic Field. For his PhD (1987–1991), Thomas joined the research group of Volker Lorenz at Würzburg University (Germany) and studied the diamondiferous Ellendale lamproites of Western Australia. Attending the 5th International Kimberlite Conference in Araxá (Brazil) in 1991 and experiencing the unique community of academics and industry geologists in that field got him hooked on mantle, kimberlite, and diamond research. A postdoctoral project on the Gross Brukkaros Caldera in Namibia still kept Thomas largely in the field of volcanology. With a Marie Curie Fellowship of the European Union, he then joined Jeff Harris at the University of Glasgow (Scotland) in 1994 where he got involved in research on diamonds and their mineral inclusions. From 1996 to 2001, Thomas was non-tenured faculty at Frankfurt University (Germany) where he worked with Gerhard Brey on diamonds and Earth mantle rocks. In 1999, he obtained his venia legendi in mineralogy and petrology. In the same year he was presented with the Victor Moritz Goldschmidt Award of the German Mineralogical Society. Thomas joined the University of Alberta in 2001, where he is now Professor and Canada Research Chair in Diamonds. Thomas’ research on diamonds initially focused on their inclusions and what they tell us about the origin of Archean lithospheric mantle and the composition of the transition zone and the lower mantle. Working with an incredible team of colleagues at the University of Alberta, he then became increasingly interested in the composition and speciation of mantle fluids and spearheaded the creation of the Canadian Centre for Isotopic Microanalysis (CCIM; funded by the Canada Foundation for Innovation), having a multi-collector ion microprobe at its heart. This enables, among other things, in situ stable isotope studies of diamonds and mantle xenolith minerals.

Hawley Medal Winners

The Hawley Medal is awarded to the authors of the best paper to appear in The Canadian Mineralogist in a given year. The award is named in honor of Dr James Edwin Hawley (1897–1965), who was a distinguished professor of mineralogy at Queen’s University (Ontario, Canada).


Zeinab Azadbakht has been the Regional Resident Geologist for the Ontario Geological Survey in the Timmins office since August 2020. After finishing her PhD at the University of New Brunswick with Dave Lentz and Christopher McFarlane, Zeinab was a contract lecturer in economic geology at the University of Regina (Canada) until she joined the Ontario Geological Survey. She has built an expertise in mineralizing systems associated with magmatism, including gold, but is expanding into critical metals research. She has a strong academic background and holds a PhD in economic geology. Zeinab has technical expertise in geoscience data compilation, igneous petrology and mineralogy, and geochronology. She has a passion for geology, adventure, and finding new and unique research projects.

David R. Lentz is the Research Chair in Economic Geology for the Department of Earth Sciences of the University of New Brunswick. He received his BSc (1983) and MSc (1986) degrees in geology from the University of New Brunswick (UNB) in Fredericton. He completed a PhD (1992) at the University of Ottawa and then worked with the Geological Survey of Canada for three years. In 1994, Lentz joined the New Brunswick Geological Survey as their mineral deposit geologist. In 1999, he won the Harvey Gross Young Scientist Medal from the Geological Association of Canada (GAC). Since 2000, he has held the Research Chair in Economic Geology at UNB, with a research focus on the petrogenesis of ore deposits. He has been a P. Geo since 2001. Dave has been honored with many awards: GAC’s Distinguished Service Award; the New Brunswick Association of Professional Engineers & Geoscientists’ Loring Bailey Geoscience Award; the Atlantic Geoscience Society’s Gesner Medal; the Canadian Institute of Mining, Metallurgy and Petroleum’s Julian Boldy Award; and the International Association on the Genesis of Ore Deposits’ International Distinguished Lecturer Award. Dave is also a Fellow of Geoscientists Canada. Notably, he has edited three popular ore deposits-related books for the Geological Association of Canada and the Mineralogical Association of Canada and has published over 300 journal articles, in addition to numerous government publications. Lentz is particularly well known for his short courses, workshops, and field trips. Currently, he is the associate editor for Journal of Geochemical Exploration, Ore Geology Reviews, Journal of Earth Science, and FACETS. He is a subject editor for the Economic Geology section of Frontiers in Earth Science.

Young Scientist Award to Dr. Anna Harrison

The Young Scientist Award is given to a young scientist who makes a significant international research contribution, and so makes a promising start to a scientific career. The areas of research considered are any, or all, subjects covered by the Mineralogical Association of Canada. The scientist will have received their PhD not more than 15 years before the award. The scientist must be a Canadian working anywhere in the world or a scientist of any nationality working in Canada. Research areas include mineralogy, crystallography, petrology, geochemistry, mineral deposits, and related fields of study.

The Young Scientist Award for 2020 went to Dr. Anna Harrison, who has a passion for geology and mineralogy. She has a strong academic background and holds a PhD in economic geology. Zeinab has technical expertise in geoscience data compilation, igneous petrology and mineralogy, and geochronology. She has a passion for geology, adventure, and finding new and unique research projects.

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The 2021 MAC Young Scientist Award and medal goes to Dr. Anna Harrison, an aqueous environmental geochemist with the CNRS (Centre National de la Recherche Scientifique, France) whose research interests broadly lie in studying the mechanisms by which elements are cycled between minerals and fluids in natural and engineered environments, and how we can harness chemical processes to limit environmental degradation.

Anna’s research has been on the potential use of mineral weathering to capture CO₂ for climate change mitigation and on understanding the fundamental mechanisms behind mineral weathering in the unsaturated zone. Recently, Anna and her colleagues have begun to explore the behaviour of non-traditional stable isotopes during mineral weathering and carbonate precipitation and its application to understanding both natural weathering and as a means to trace captured CO₂. She received her BSc from the University of Alberta (Canada) and, in 2015, her PhD from the University of British Columbia (Canada). She was a postdoctoral fellow at Stanford University (California, USA), an NSERC postdoctoral fellow at Geoscience Environment Toulouse (a part of the CNRS), and a Marie Skłodowska-Curie Fellow at University College London (UK). Anna was an assistant professor in environmental geochemistry at Queen’s University (Canada) before returning to France to join the CNRS.

**Berry Medal to Mr. Malcolm Back**

The Leonard G. Berry Medal is awarded annually for distinguished service to the association. The award recognizes significant contribution to the association in one or more areas that may include leadership or long-term service in an elected or appointed office, or making important contribution(s) that enhances the mineral sciences in Canada or that broadens the Canadian mineralogical perspective. The medal is named after Leonard G. Berry (1914–1982), a founding member of the MAC, editor of *The Canadian Mineralogist* (and its predecessor) for 25 years, and the first winner of the MAC Past-Presidents’ Medal.

This year’s awardee is Mr. Malcolm Back, a retired research assistant in the Department of Mineralogy at the Royal Ontario Museum.

Mr. Back received his BSc in 1985 from the University of Toronto (Canada) and his MSc in 1990 (“A Study of Tellurite Minerals: Their Physical and Chemical Data Compatibility, and Structural Crystallography”) from the same institute. He began his mineralogical career as a research assistant in the Department of Mineralogy at the Royal Ontario Museum (ROM) in 1985, with a focus on X-ray diffraction; he retired from this position in 2011. He worked under the tutelage of Joe Mandarino, Fred Wicks, and Robert Gait at the ROM, developing the knowledge and skills necessary to become the mineralogist he is today. Mr. Back has had a life-long interest in tellurium oxysalt minerals and, in recognition of his contributions to mineralogy, and specifically tellurium oxysalts, the new species backite, Pb₂Al₂(TeO₆)₂Cl, from the Grand Central Mine of the Tombstone Hills (Arizona, USA) was named in his honor. Mr. Back is a volunteer par excellence, offering his time freely and without reservation to many amateur associations (e.g., serving several times as President of the Walker Mineralogical Club, and providing mineral identifications at the Bancroft Gemboree). Mr. Back has been maintaining and continuing to ensure the publication of the indispensable Fleischer’s *Glossary of Mineral Species*. This small, relatively nondescript volume, is an indispensable resource for active mineralogists working on new or rare minerals, as well as those seeking to appreciate how diverse the world of mineralogy is. He began his work on the *Glossary* in 2004, with the late, great, Joe Mandarino as senior author. After Joe’s far-too-soon passing in 2007, Mr. Back immediately assumed the role of senior author, a task which he continues to this day. He also continues to work on Joe Mandarino’s unpublished *Encyclopedia of Minerals*, with the hope that one day, this too will be brought to light.

**OBITUARY**

**IN MEMORY OF GAIL E. DUNNING (1937–2021)**

Gail Dunning, the 2020 recipient of the MAC’s Pinch Medal, recently passed after a courageous battle with lung cancer. He was first hired in 1959 as a chemist at General Electric’s Nuclear Energy division (San Jose, California, USA), transferring five years later to the position of metallurgist, specializing in failure analysis. He was an avid, eager field collector, with a sharp eye and mind that he initially applied to unusual minerals (e.g., pabstite) and later, to the geology and mineral paragenesis at such localities as the Kalkar quarry (Santa Cruz County, California, USA), the Big Creek-Rush Creek-Trumbull Peak Bₐ-silicate belt (Fresno and Mariposa Counties, California, USA), the Clear Creek Mine and Claim (San Benito County, California, USA) and the McDermitt Mine (Humboldt County, Nevada, USA). Gail was not just a mineral collector, but an individual who, with his inseparable companion Fen Cooper, documented their observations and findings which were then published as scientific communications (> 40) in journals such as *Mineralogical Record*, the *American Mineralogist* and *The Canadian Mineralogist*. He possessed a scientifically astute mind, which led to his involvement in the discovery of >10 new mineral species, all coming from collaborations with internationally recognized, professional mineralogists who equally held him in high regards. He amassed a collection of > 5,300 specimens representing 4,000 species, the majority of which were self collected. His >55 years of contributions to the mineralogical realm were recognized with the publication of the new mineral species, gaildunningite (a Hg nitride, from the Clear Creek Claim in San Benito County) in 2019, and by being the 2020 Pinch Medal recipient. Gail was a special person who was always willing to share his mineralogical knowledge, skills and passion with anyone, regardless of their background or age. He was an inspiration to many and while he will be missed, he will never be forgotten.

**Andy McDonald**

Harquail School of Earth Sciences
Laurentian University
Ontario, Canada
EDITORIAL

The Peer Review System is at Risk. We Need You to Defend It!

My previous editorial addressed the cost of publishing in open access and the different open access business models. In the present editorial, I will focus on the peer review system: its current challenges and risks.

Due to the large increase in the number of submitted manuscripts, it is more and more challenging to find dedicated reviewers for all these manuscripts. Imbalances between “supply and demand” creates conditions for aggressive competition and for new approaches to appear. There are discussions on the idea of paying reviewers for their work. Some journals have already started providing compensation to some reviewers in the form of free publications. These journals are competing with others that can only ever have a voluntary peer review process. Such a situation is extremely dangerous and could rapidly become uncontrollable. First, a contribution to reviewers removes the transparency of the financial model of scientific publications, which scientists are just now starting to attain through the open-access system. In addition, this practice will, ultimately and inevitably, result in an increase of publication costs ... because someone has to pay for this!

There are more fundamental reasons that justify isolating the review system from any commercial practice. Up to now, authors from each discipline review each other’s work. In fact, I would even call it a “community review” rather than a “peer review”. If we begin to pay, or somehow financially reward, the reviewers, there is a risk that the community could progressively split into two: authors (with enough money and who publish a lot) and “professional reviewers” (who publish more rarely or even not at all). It is important to counteract this trend and to keep the review process in the hands of authors (i.e., those active in the scientific community), so maintaining a fully “community” review system.

Another risk that authors face when having to sign a reviewer’s agreement or contract with a publisher in return for any form of reward is the loss of freedom attached to any contractual commitment. Publishers, who are usually the owners of the journals, may put high-demand on the rapidity and efficiency of the review process. To decline a request for a review, even if with a short deadline, may be difficult when an agreement has been signed and any future reward may be lost. Currently, some publishers are already setting less than two weeks as the deadline to reviewers. Contracted reviewers are expected to follow the publisher’s policy or renounce the contract (and its inherent rewards).

As we know from many systems involving two groups with different financial models, those offering rewards or payment get advantages, including loyalty and a consequent stronger influence (in the market). Once a commercial review system is launched, there will be a race between publishers to attract and retain the best reviewers, which may create an inflation on the level of payments. In this scenario, it is unlikely that the most ethical or equitable journals – including journals of small, learned societies – will have a fair chance in this battle. The large commercial publishers, and publishers involved in mass-production, have all the chances to win the competition. It will be increasingly difficult for publishers that want to keep the free “community review” approach to find reviewers wanting to spend time to review articles for free. The two systems cannot survive together.

The European Journal of Mineralogy, along with most other journals owned by learned societies, provides no reward or payment to its editors or reviewers. We believe it is important to defend the free voluntary-based review system as the only one able to guarantee transparency, fairness, and quality in the evaluation.

But without the strong support of its community members, the learned societies alone will not be able to maintain this system for long.

It is a simple calculation. To function, the review system needs to ensure that there are at least two times more reviews than the number of submitted papers by any given (every) scientist. This means that authors must review at least as many papers as they publish, but preferably twice as many (to account for multi-author papers on one side and rejected papers on the other side). We can consider it a “scientific civic duty” for each author to contribute to the review system and its sustainability. Part of this duty is to accept review invitations independent of the manuscript’s quality, assuming we feel scientifically competent. To meet the reviewing needs, it is also crucial to involve more junior scientists. Senior scientists have a major role to play by providing more reviewing opportunities to more junior colleagues (e.g., through nomination, support, etc.). As senior scientists, we have the responsibility of engaging the younger ones in understanding the importance of reviewing as a vital part of one’s scientific community duty.

Only together and united can we aspire to keep the free “community review” alive. The publishing system does not exist without authors. We, the authors, have tremendous power! It is our responsibility as authors to decide which publishing system we want and then to act in agreement with our convictions!

Jannick Ingrin
Managing Editor of EJM
MESSAGE FROM AAG PRESIDENT DENNIS ARNE

The start of 2021 brings us five council members to the Association of Applied Geochemists, each of whom will serve two-year terms from 2021 to the end of 2022. They are as follows:

Patrice de Caritat (2nd term), Dave Heberlein (2nd term), Ryan Noble (1st term), Pim van Geffen (1st term), Paul Morris (1st term).

I would like to thank Patrice and Dave for standing for another two-year term, and Ryan, Pim, and Paul for agreeing to serve on council. For Ryan and Paul this will be their second time around, as well as having served as past presidents. The important work of running the AAG is done by council and its various committees. I would encourage Fellows to stand for nomination for the period 2022–2023, and Ordinary Members to upgrade to Fellow status so that they can stand for council and help determine the future direction of the AAG.

I would also like to congratulate Dr Robert (Bob) Garrett for being awarded an Honorary Fellowship: this followed a formal nomination by his peers, approval by the Awards and Medals Committee, and ratification by council. Bob is only the eighth AAG member to ever receive such an honour, and he joins Gwendy Hall as the only other current Honorary Fellow. Both are deserving recipients for their long service to our profession.

It is also my pleasure to congratulate Professor Cheng Qiuming as recipient of the AAG Gold Medal for 2020. Qiuming is the founding director of the State Key Lab of Geological Processes and Mineral Resources at the China University of Geosciences (Beijing). The Gold Medal is awarded for outstanding scientific contributions and achievements in applied geochemistry.

The AAG and the International Association for Mathematical Geosciences (IAMG) have formally signed a memorandum of understanding between the two societies to foster cooperation. There is already some cross membership between the two societies and there is much to be gained through further interaction. One benefit is that each society can contribute to each other’s newsletters, so if any AAG members have suitable content please contact the editor, Katherine Silversides, at newsletter@iamg.org. Thanks goes to John Carranza for pushing this along.

In other news, the Society for Geology Applied to Mineral Deposits (SGA) has announced the postponement of their 16th biennial meeting in Rotorua (New Zealand) from November 2021 to a new date of 28–31 March 2022. The AAG is a co-host of the conference and has agreed to sponsor an exploration geochemistry workshop (Wahid Salama is the coordinator) and a session on spatial data analysis for mineral exploration (Dr Arianne Ford and Dr John Carranza are the co-convenors). We hope that international travel restrictions to New Zealand will have eased sufficiently by then for the conference to be well attended.

We have also submitted a proposal to the Australasian Exploration Geoscience Conference (AEGC) to conduct a two-day short course in exploration geochemistry at their conference in Brisbane in September 2021. As the conference is of local interest, and there is potential for a travel bubble between Australia and New Zealand later this year, we hope that this conference may proceed with a live venue and that the AAG will have several members there to contribute to the short course.

Which brings me to the International Applied Geochemistry Symposium (IAGS) scheduled for later in 2021. The local organizing committee, under the guidance of Brian Townley, has been keeping a close eye on the roll-out of vaccines in Chile. Vaccines are well advanced on a global scale, but there are concerns that international travel restrictions, not to mention budgetary constraints, will limit attendees in person. For these reasons, we are planning a hybrid model for the conference that would allow participants to join live sessions online. This is likely to be a model going forward for future symposia, given the advances in both the technology and our recent acclimatization to its use. The local organizing committee has further suggested that we consider postponing the IAGS for another year, instead holding it in October 2022 to ensure that as many people as possible can attend. The AAG Executive are in favour of this suggestion and council will discuss this at their March meeting. A formal announcement will be made in due course.

OBITUARY FOR EDWARD (“ED”) DRONSEIKA (1953–2021)

Exploration geochemistry has lost a real character with the death of Ed Dronseika on February 24 in Perth (Australia) [All locations herein are Australia unless otherwise stated]. Ed was a great enthusiast in all that he did. He was a passionate geochemist and a lateral thinker who often had a refreshingly different and interesting perspective on topics. He was inquisitive and never afraid to ask questions – many of us will recall being held to account by Ed if we were not able to fully explain our theories.

He was a pioneer in commercial laboratory partial digest methods, and he became a world-leader in this field. His success was due to his quest to understand the mechanisms by which processes happen and his willingness to experiment, adapt, and continually learn.

Ed was born in Melbourne and studied geology at Royal Melbourne Institute of Technology (RMIT) in the early 1970s. He worked as both a mine and exploration geologist in what is now Zimbabwe and Namibia in the late 1970s before returning to Australia to work for a decade on the west coast of Tasmania. He worked on tin at the Cleveland Mine, and then with Aberfoyle Ltd on the polymetallic volcanicogenic massive sulfide deposit of Que River. He spent most of the 1990s in Queensland working for Aberfoyle Exploration, first at Charters Towers and then in Townsville. Ed was responsible for exploration in the Mt Isa region, where he discovered several new prospects.

In 1998, he started specialising in the emerging field of partial digest geochemistry to create cost-effective methods for exploration under cover. After consulting with Terrasearch Ltd in Townsville on these methods, he was recruited by Genalysis Laboratory Services (now Intertek Genalysis) in Perth to work with Chief Chemist Ann Evers to set up what has become the successful and well-known suite of TerraLeach™ partial digests.

Ed continued to improve his methods and their applications in exploration by working closely with his many clients at Intertek Genalysis, with considerable success in several parts of Australia and Africa in particular. He built a close-knit team in the Partials Lab at Intertek Genalysis, and it is hoped that his work will continue in the capable hands of Irene Patchett, his second-in-command, who has kept the “show on the road” during Ed’s recent period of illness. Ed was a vibrant, multi-skilled person and knowledgeable on many topics, including wine. He was a regular at geology and geochemistry events and was generally a great bloke and lots of fun to socialise with.

The geochemistry and geochemistry community extends their condolences to Ed’s family, especially his wife Elizabeth, son Anton, and daughter Kate.

Please raise a glass (or two) to the one and only Ed Dronseika. He will be missed by all.

Helen Waldron and Ann Evers
The COVID-19 pandemic has considerably, and adversely, affected the training and career development opportunities for junior scientists over the past year. Sadly, it continues to do so in many regions. While we all eagerly anticipate the return of in-person conferences and meetings, we are still in uncertain times. Nevertheless, the European Association of Geochemistry (EAG) is continuing to increase its efforts to support early career scientists by adapting its three key initiatives (see below) to aid participation in all types of events, whether in virtual, hybrid, or in-person format.

Whatever format of event you are planning to attend or organize, visit https://www.eag.eu.com/early-career/ to find out more and to apply!

**STUDENT SPONSORSHIP PROGRAM**
This program sponsors up to 12 students each year to participate in virtual, hybrid, and online conferences, short courses, or summer/winter schools. For in-person events, the events should be held in Europe, but events may be hosted anywhere if students intend to participate online only. Sponsored students are awarded up to €500 to cover registration/abstract fees and, if applicable, travel expenses.

*Application deadlines: 1 February, 1 May, 1 September, and 1 December*

**EARLY CAREER SCIENCE AMBASSADOR PROGRAM**
Originally aimed at early career scientists based in Europe who wished to attend in-person at a conference held outside Europe, this program has recently been expanded to welcome applications from early career scientists from any country to attend virtual conferences hosted anywhere in the world. The program aims to fund conference attendance, not related events such as field trips. To be eligible, applicants must intend to present their work at the conference. For online attendance, successful applicants will receive awards covering registration and abstract fees. For in-person attendance, successful applicants will be awarded 50% of expenses (travel, registration, and abstract fees) up to a maximum of €1,500.

*Application deadlines: 1 March, 1 June, and 1 October*

**SHORT COURSE AND CONFERENCE SPONSORSHIP PROGRAM**
If you are an EAG member and are organizing a short course or small conference in Europe (whether online, hybrid, or in-person) you can apply for EAG Sponsorship to support student participation. Successful applicants receive sponsorship of to up to €200 per student. Short courses or small conferences should focus on special topics or techniques from the broad field of geochemistry.

*Application deadline (for events taking place in 2022): 30 November 2021*
THE PRESIDENT’S CORNER

My year-long presidency of the Clay Minerals Society (CMS) is soon coming to an end. By the time you read this President’s Corner, Jeffery A. Greathouse (Sandia National Laboratories, New Mexico, USA) will be our next president. Looking back over the past year, I am reminded that it was essentially driven by the question, “How can we cope with the pandemic?”

We have all been dealing with this pressing question from personal and professional points of view, trying to minimize the overlap between these two “lives”. This could be quite challenging when mostly working from home and/or under lockdown and travel restrictions that minimized social interactions down to a shrunken core of close relatives. This situation made the availability of various vaccine solutions now offers the prospect of a “back-to-normal” life. Such normalization is especially welcome in terms of increased socialization, face-to-face exchanges, discussions, or even scientific arguments.

Yet, the COVID-19 pandemic has also offered a fantastic opportunity to escape from our usual routines and to reinvent ways to collaborate and interact. There may be limitations, to be sure, but these alternatives may release some constraints on time and travel and allow for faster and more efficient interactions, especially within existing collaborations and/or for small group meetings.

For learned societies, the pandemic has also been a time to reinvent their relationship with their members. This has largely been achieved by broadening what societies can offer using available technology and a worldwide access to the Internet. Remote attendance of conferences offers a cheap and more eco-friendly access to current scientific developments and knowledge. Remote access also means that developing countries have better access to scientific developments where previously there was insufficient funding or travel restrictions to attend regular conferences. Logically, diversification of our activities should aim to include more e-communication to enable remote attendance to conferences, webinar series, and a stronger presence on social media. In 2021, the CMS annual meeting will be organized as a fully on-line workshop entitled Clay Minerals in Healthcare Applications. Details are available at https://www.clay.org/2021-meeting-2/.

In all cases, the primary driving force for a society’s vitality and activity is that of its members, and I hope the information regularly published in these pages will incite you to start, renew, or maintain your membership in the Clay Minerals Society. Before leaving the president’s gavel to Jeffery, I would also like to thank all members of the various CMS committees who tirelessly devote their time and expertise on behalf of the society. Special thanks are due to two members of the CMS Executive Committee who are stepping down from their long-term commitments: Secretary Warren Huff, who had been in that role for 15 years and is one of the very few members who joined the CMS at its official creation in 1963; and Treasurer Paul Schroeder who has served in that role for the last 6 years after acting as president (2010–2011).

Bruno Lanson (bruno.lanson@univ-grenoble-alpes.fr)
President, The Clay Minerals Society

VIRTUAL CMS MEETING FOR 2021

Our annual meeting, the International Clay Conference, which in 2021 was to have been in collaboration with colleagues in Turkey, has been postponed to 2022. Thus, in the interim, we have decided to hold a two-day virtual workshop: the International Workshop on Clay Minerals in Healthcare Applications. The workshop will be based on the two special issues of Clays and Clay Minerals entitled “Clay Minerals in Health Applications” and “Clay Minerals in Healthcare”, which are to be published in 2021, and the workshop will also incorporate contributions by colleagues from the Qing Yang Institute for Industrial Minerals (China). Sessions will be organized by Eduardo Ruiz-Hitzky (of the Materials Science Institute, Madrid, Spain) and Chun Hui Zhou (of the Qing Yang Institute).

Speakers confirmed so far, and their talk themes, include:

- Lynda Williams and colleagues: Evaluating in vivo applications of a natural antibacterial clay to wound infection
- Pilar Aranda, Ruiz-Hitzky and colleagues: Clay-based bionanocomposite films for wound dressing applications
- Bernard Lopez and colleagues: Response of mammalian cells to interaction with sepiolite
- Giora Rytwo and colleagues: Health protection using clay minerals: a case study based on the removal of BPA and BPS from water
- Yuri Lvov: Halloysite nanotube vehicles for drug delivery through brain endothelial barrier
- Rawil Fakhruilin and colleagues: Self-assembly of halloysite nanoclay for hair surface engineering
- Ana Alcântara and Vera Constantino: Layered clays as versatile nanodevices to drug delivery systems
- César Viseras and Alberto Galindo and colleagues: Clays in cosmetics and personal care products

There is no registration charge for members of the Clay Minerals Society, but non-members will be asked to pay a modest fee.

DECEMBER 2020 ISSUE OF CLAYS AND CLAY MINERALS

“Laterite as a potential seepage barrier from a karst-depression tailings impoundment” – Hai-Yan Gao, Ze-Min Xu, Zhe Ren, Kun Wang, Kui Yang, Yong-Jun Tang & Jun-Yao Luo

“Genesis of palygorskite in the Neogene Baiyanghe Formation in Yangtaiawan basin, northwest China, based on the mineralogical characteristics and occurrence of enriched trace elements and REE” – Shuai Zhang, Li Lihui, Qinfei Liu, Bingjie Zhang, Zhihuan Qiao & Brian J. Teppen

“Automated full-pattern summation of X-ray powder diffraction data for high-throughput quantification of clay-bearing mixtures” – Benjamin M. Butler and Stephen Hillier

“Clay mineralogy of surface sediments in the Three Gorges Reservoir: implications for sediment provenances and weathering regimes” – Shuai Wang, Wenbo Rao, Jin Qian, Mengying He, Changping Mao, Kun Li, Yuexing Feng, and Jianxin Zhao

“Mineralogy, geochemistry, and genesis of kaolinitic claystone deposits in the Datong coalfield, Northern China” – Linsong Liu, Qinfei Liu, Thomas Algeo, Hao Zhang, Yongjie Yang, Gaoyu Peng, Shuai Zhang, Hanlie Hong & Di Liu

“Preparation and characterization of halloysite-based carriers for quercetin loading and release” – Shu-Ting Liu, Xue-Gang Chen, Shi-Long Zhang, Xue-Min Liu, and Jun-Ji Zhang

“Developing an efficient catalyst based on thermal and acid-treated clay for the removal of trace olefins from aromatic compounds” – Nooshin Nouri, Mahboubeh Tasviri, and Hossein Ghasemzadeh

“Functionalized halloysite nanotubes for enhanced removal of Hg2+ ions from aqueous solutions” – Salvatore Cataldo, Francesco Crea, Marina Massaro, Demetrio Milea, Alberto Pettignano, and Serena Riela

“Optimization of hydrogen generation by catalytic hydrolysis of NaBH4, with halloysite-supported CoB catalyst using response surface methodology” – Seda Hosgum, Mine Ozdemir, and Yeliz Buruk Sahin

“Fabrication of anthocyanin/montmorillonite hybrid pigments to enhance their environmental stability and application in alcloroic composite films” – Shu E. Li, B. Mu, Jun J. Ding, H. Zhang, Xiao W. Wang & Ai Q. Wang

“In Memoriam: Peter Komadel”

Go to https://link.springer.com/journal/42860/volumes-and-issues to see the latest issues.
The first year of publication by open access has been finished with volume 32 of the European Journal of Mineralogy (EJM). Some statistics may help to see where we are right now. Altogether, 53 papers were published. Based on the extrapolation of the current submission rate, we can expect many more papers in 2021. Acceptance was 75%, and the time between the final decision by the editorial board and publication of an article decreased to a median value of 26 days—a significant improvement! Reviewers needed, on average, three weeks to submit their reviews (i.e., the required time in the editorial system), and, considering the time needed to write a thoughtful review, we should not demand shorter periods. Some 62% of the papers are from members of the owning or associated national societies (those of Spain, France, Italy, Germany, and the European Association of Geochemistry), and currently for 2021 this is in the same order of magnitude. The EJM is a truly international journal: 22 countries are mentioned in the article affiliations, with first authors from Germany and Italy (16% each), China (11%), France and Russia (9% each), and the USA (6%).

Attention PhD students! There is a special offer for PhD students who are members of the DMG. For one paper from your PhD thesis, the DMG will sponsor the article processing charges (APCs). The procedure is simple: once your paper is accepted, please pay the APCs and send us the receipt together with a confirmation letter from your advisor that you are a PhD student. And some additionally important information for everyone: Copernicus will directly ask your university/institution, when you submit your paper, for the charges; many institutions will have a contract by which the APCs are paid.

A forthcoming special issue of the EJM will be entitled “Mineralogy of the Built Environment” and will be edited by Carlos Rodriguez-Navarro, Gilberto Artioli, Maria Chiara Dalconi, and Kerstin Eierl. Submissions commenced on 1 April 2021 and will remain open until 1 April 2022. The study of materials used in the built environment has long attracted significant research efforts and has only grown in popularity over the last few decades. Mineralogy has been pivotal in these studies, from the analysis of the different mineral components of natural stone and earthen structures, the composition of man-made plasters, mortars, cements, and ceramics (bricks), to the weathering and conservation of the aforementioned materials. Studies should focus on both traditional and novel materials used in the protection and conservation of built heritage, including, but not limited to, lime-, silica-, oxalate-, and phosphate-based materials (e.g., nanolimes and alkoxysilanes). We seek studies that have a focus on the following:

- The analysis of natural and man-made building materials. In particular, studies on the analysis of minerals/phases of different building materials, the phase evolution in cementitious materials (e.g., during processing and setting of lime mortars, gypsum plaster, or cement/concrete), and ceramics (e.g., phase evolution during firing of bricks).
- Mineralogical changes that occur during physical and chemical weathering, as well as during biodeterioration. In particular, the mechanisms that lead to degradation and that involve a phase transformation (e.g., dissolution and precipitation), and/or neoformation (e.g., salt weathering), and clay-related damage (i.e., swelling and shrinking).

- The mineralogical analysis of inorganic conservation materials, their applications, and an evaluation of their effectiveness.

Another new special issue about glass/melt inclusions in igneous and metamorphic rocks is in preparation: the editors will be Elisabetta Rampone, Sylvio Ferreiro, and Marie Edmonds. If you are interested in contributing, please contact the editors or François Holtz for further details.

Gerhard Franz (Berlin)

JOINT DMG–MINERALOGICAL SOCIETY OF AMERICA VIRTUAL SHORT COURSE REPORT

Application of Diffusion Studies to the Determination of Timescales in Geochemistry and Petrology

Short course held 19–23 April 2021 at the Institute for Geology, Mineralogy and Geophysics of the Ruhr University Bochum

Dr Sumit Chakraborty and Dr Ralf Dohmen of the Institut für Geologie, Mineralogie und Geophysik, Ruhr-Universität Bochum (RUB) (Germany) ran the workshop Application of Diffusion Studies to the Determination of Timescales in Geochemistry and Petrology. This workshop was a great success and ended 23 April after a week of inclusive lectures and practical sessions. Despite being postponed from October 2020 and held virtually on Zoom (due to the COVID-19 pandemic), the organizers still managed to delicately deliver the art of diffusion modeling from top to bottom to a group of 53 participants from 18 countries, including North America, Europe, Asia, South America, and Africa, the participants being at various stages in their careers.

Some of the participants at the joint MSA–DMG shortcourse on diffusion modeling, held on Zoom.

Diffusion chronometry and geospeedometry have been applied to a wide range of igneous and metamorphic systems to obtain timescales which further shed light on the pace of petrological processes. Within the six-hour window of the course each day, the short course started from basic concepts and the mathematics of diffusion and gradually moved to more advanced topics and areas of active research, including multicomponent diffusion and moving boundary conditions. The lecturers also kindly shared their tips and tricks alongside common mistakes they have encountered on diffusion modeling. “Your model is only as good as how well you understand your petrological system” was one of the most critical take-home quotes from Sumit’s lecture. Although easily overlooked, the petrographical and geological contexts are the key sources of information when setting up a model.
Interspersed between lectures were five well-designed practical units that allowed participants to apply the learned concepts and numerical tools to model natural diffusion processes on their computer. The participants were divided into five groups to facilitate discussion and collaboration; one of the following was responsible for each group: Jennifer Primocerio, Thilo Bissbort, Sampriit Basak, Priyadarshi Chowdhury, Ralf Dohmen. Other than Ralf, all are early career scientists associated with the Bochum group. The practical units started from modeling diffusion processes using analytical solutions and then finite-difference models in Excel spreadsheets. Then we moved on to create models with composition-dependent diffusivities and learned how to code that into Matlab. The workshop ended on Friday with a big Zoom photo and the lecturers generously providing time for one-on-one discussions.

Although the online setup this year precluded social events – happy hours, networking, and laboratory tours – the workshop still provided an informative and solid introduction for scientists who were interested in applying diffusion chronometry to their research. Special thanks go to the DMG, the MSA, the organization team, and all the teachers from the RUB group for making such a splendid event available during the COVID-19 pandemic.

Kuan-Yu Lin (University of Delaware, USA)
The Geochemical Society (GS) seeks to celebrate and share outstanding achievements in geochemistry through our awards and special lecture program. To do this, we need your help in recognizing the innovative scientists who are making major contributions to the field.

Anyone (with the exception of those involved in the award selection process) may submit a nomination. This includes early career and more senior scientists. Considerable progress has been made regarding the diversity of nominees in recent years, but more progress is still needed. The cultural richness represented by GS members from 70 countries should also be reflected in the awards that we grant for scientific achievement. This is important not only in the interest of equity but also to ensure that all the young scientists who participate in the society and who attend Goldschmidt conferences recognize their potential future selves in the persons being honored.

Please consider submitting a nomination in 2021 by the October 31 deadline. Information on how to submit an award nominations package can be found at the GS’s website: www.geochemsoc.org/honors. Nominations of people from underrepresented groups are encouraged (e.g., women, non-white researchers and/or researchers from Asia, Africa and Latin America, disabled scientists, those who have led diversified careers, other historically minoritized groups, and intersections thereof).

The society is accepting nominations through October 31 for the following awards:

The V. M. Goldschmidt Award is the society’s highest honor. This award is presented annually for major achievements in geochemistry over a career. Beginning this year, the definition of major achievement has been significantly broadened. Full details are on the website.

The C. C. Patterson Award recognizes an innovative breakthrough of fundamental significance in environmental geochemistry, particularly in the service of society, consisting of either a single outstanding contribution or a short series of papers published within the last decade.

The F. W. Clarke Award recognizes an early career scientist for a single outstanding contribution to geochemistry or cosmochemistry, published either as a single paper or as a series of papers on a single topic. To be eligible, a candidate must have received a recognized doctorate or its equivalent within seven years of 1 January 2022. (Beginning this year, age is no longer taken into account.)

The Alfred Treibs Award, presented by the Geochemical Society’s Organic Geochemistry Division, is given for major achievements, over a period of years, in organic geochemistry.

The John M. Hayes Award, created in 2017, is given by the Organic Geochemistry Division to a mid-career scientist for outstanding accomplishments that draw together multiple fields of investigation to advance biogeochemical science. The awardee will be selected based on innovative research which lies at an intersection of isotope geochemistry, organic geochemistry, microbial ecology, biogeochemistry, astrobiology and/or analytical innovation.

Joint GS–EAG Geochemistry Fellows. In 1996, the Geochemical Society and the European Association of Geochemistry established the honorary title of Geochemistry Fellow, to be bestowed upon outstanding scientists who have, over some years, made a major contribution to the field of geochemistry.

The society is also accepting nominations for special lectures, which will be presented at Goldschmidt2022 in July 2022. Lecture nomination packages are relatively short, requiring only information about the nominee and one letter of support. A single nominator can easily assemble a package. The lectures are featured prominently at Goldschmidt and are a great way to share a colleague’s exciting work with attendees.

The Robert Berner Lecture, a joint program of the Geochemical Society and the European Association of Geochemistry, is given annually by a mid-career scientist. The lecture is on a “Berner” subject, which includes a wide range of topics associated with elemental cycling at the Earth’s surface (molecular to planetary scale, modern to ancient oceanic and terrestrial systems, evolution of the biosphere, etc.).

The Endowed Biogeochemistry Lecture recognizes a prominent scientist who is making cutting-edge field-based measurements or laboratory measurements on field samples in the area of biogeochemistry.

The F. Earl Ingerson Lecture honors the Geochemical Society’s first president. Nominations are accepted for any topic within geochemistry that will have a broad appeal to Goldschmidt attendees.
The Geochemical Society is committed to increasing diversity in geochemistry and among its formally recognized inspirational and prominent figures. We seek to promote and encourage diversity and inclusion while furthering equity, a true sense of belonging, and success for all people. In particular, the society is keen to encourage talented researchers from underrepresented groups to serve as nominators, and to be nominated for society awards. Below is information that may assist potential nominators.

**What is “geochemistry”**?
“Geochemistry”, broadly defined, is the study of the chemistries of and the processes in the solid Earth (and extraterrestrial bodies), atmospheres, hydrospheres, and biospheres. The development of new geochemical tools and instrumentation is also award-worthy.

**Who can submit a nomination?**
Any member of the geochemistry community may submit a nomination, except for the current GS Board of Directors and people serving on the selection committee of the award. Membership of the society is not required.

**Who can be nominated?**
Any Earth scientist making major contributions to geochemistry can be nominated. Society membership is not required. Nominators should have a track record commensurate with continued adherence to the conduct expectations of the society (please refer to Geochemical Society’s code of ethics). In particular, there should be no documented violation of these codes on record.

**How do I nominate someone?**
Each award has its own requirements, but all require a letter from you (the principal nominator) describing how the nominee meets the award criteria. A short version of the nominee’s curriculum vitae (CV) and a list of their publications is also needed. Some awards require a second letter, which can be signed by several people. These materials should be submitted electronically via the GS website by the annual nomination deadline. To find the requirements for every award, visit https://www.geochemsoc.org/honors.

**Does my nomination have a chance of success?**
Yes! Most named awards have about 5 nominations per year, and we would like to increase this number. The Geochemistry Fellows Honor receives the most nominations (more than 80 were considered last year). The unsuccessful nominations for many awards are carried over for three years and considered again in subsequent years.

**Who selects the award winners?**
Each award has a committee between 5 and 8 members, each of whom serves a three-year term. These committees are international, diverse, and multidisciplinary. The award committee makes a recommendation to the GS Board of Directors, which makes the final decision on the recipient.

**What factors does the committee use to determine who gets an award?**
The full criteria for each award can be found on our website by selecting the particular award.

**OK, I read the criteria on the website, but what other criteria are actually used?**
There are no secret criteria! Committees are asked to make holistic assessments of nominees’ contributions based only on the criteria listed on the website.

**What processes are in place to ensure fairness?**
Each committee must follow a set of best practices in its deliberations. Award committees also submit reports to the Board of Directors after their deliberation detailing the processes used to arrive at the final decisions. The Board of Directors has oversight and the final say on awards.

**Are metrics like H-index important?**
Single metrics such as H-index have many drawbacks, including that they are not translatable between disciplines or even between geochemistry sub-disciplines. Thus, committees are discouraged from placing too much weight on any given metric. A nominee’s publications are often an important component of the evaluation, but the content and significance of the person's contributions are more heavily weighted than any single metric.

**How is the Geochemical Society trying to recognize a more diverse range of scientists?**
The Award Nominations Committee actively seeks a diverse pool of nominations by encouraging members of the community to submit them. Membership of the selection committees is diverse in terms of nationality, gender, field of expertise, and other factors. The committee emphasizes the diversity of excellence as a goal of all awards. In the last few years, the society has rewritten the criteria for some awards to include contributions that create a dynamic environment essential for scientific progress, including building infrastructure and significant contributions toward greater diversity, equity, and inclusion (DEI) within the discipline.

Review of awards criteria is ongoing with the aim of recognizing a more diverse range of scientists and contributions within geochemistry.

**Will I receive specific feedback about my nomination?**
We will notify you whether your nominee is selected or not. The selection committees cannot provide specific feedback about nominations. Nominations are considered active for three years, so those not selected are automatically rolled over to the next year (provided they still meet the criteria).

**My question is not on this list.**
Please send an email to awards@geochemsoc.org and we will be glad to answer it.

**GS Introductory Student Memberships**
To increase student participation, the GS grants free memberships to students in countries that are underrepresented in the society. This includes most countries in Africa, Asia (excluding China, Japan, and South Korea), and Central and South America. Introductory Student Memberships offer benefits including print and online subscriptions to *Elements*, the weekly *Geochemical News* e-mail, and discounted registration rates for the Goldschmidt Conference and other scientific meetings. More information is available at https://www.geochemsoc.org/programs/ism.
Why be a Member of the MSA?
I write this, my fourth President’s Letter, in mid-April 2021. Things are looking up, at least in the US, regarding the pandemic. The federal government once again respects science and makes policy decisions accordingly; vaccinations are becoming available and, at least where I live, there is little hesitation in taking advantage of that availability. Of course, things are not yet back to “normal.” Meetings are still being morphed into virtual extravaganzas and there are advantages to that format. There are also disadvantages. Attendees listen to talks more, as the option of milling around and talking about hiking, where to eat and what to drink, has all but vanished. However, the positive social and research consequences of milling about—new collaborations, a discovery of common interests, and all the other serendipitous aspects of social interaction—are gone. Of necessity, research presentations are recorded, often prerecorded, and are available to watch at one’s leisure. No more rushing from room to room hoping to catch a talk only to discover that the Chair has lost control of the schedule and thrown everything into disarray. These alternatively structured meetings are perhaps more civil and, arguably, more civilized. Is that a good thing? Will the research meeting of the future be forever changed and emerge as a hybrid of what necessity forced upon us? I suspect that it will, and I think that is a good thing, because it forces us all to reevaluate how we do business and whether the traditional practices are still the most effective way to best communicate our science.

The Mineralogical Society of America (MSA) is about to have its second council meeting for 2021, and many of us in leadership are thinking about how to better address the needs of members. The society journal (American Mineralogist), Elements, short courses, the Reviews in Mineralogy and Geochemistry volumes, our lecture program, and grants to support student research are the primary benefits of MSA membership. Although the MSA does not sponsor its own annual meeting, we participate in the annual meetings of other societies and contribute significantly to these by mounting short courses and sponsoring sessions. With the exception of the direct research grant awards, all of these benefits are generic; nonmembers benefit to almost the same extent as members. As a consequence, membership of the MSA tends to be more motivated by loyalty; sustained membership perhaps in part by inertia. Surely, the silver pin at the end of 25 years and the gold one at the end of 50 years is not reason enough to keep paying those yearly dues? And, demonstrably, many early career researchers feel that way, because they constitute the demographic shallow end of the MSA membership pool. Are there ways that the MSA can address the tangible personal benefits of membership? Can we attract more early career researchers and engage its members directly? Personally, I have memberships in three scientific societies. They all treat me in about the same way: that is, they largely ignore me and I pay my dues. I maintain these memberships in one case to receive abstracted meeting fees, and in the two other cases for nostalgia: I joined as a graduate student and kept it up until now. In one case, I am getting very close to that gold pin. I think that my motivation for membership should not be the reason that others join the society or maintain their memberships. What do you think? Isn’t it time to ask the question of what can society membership do for you? Let me know what you think. I would like some feedback on this issue.

As always, stay safe and stay healthy,

Mark Ghiorso, 2021 MSA President

2020 MSA ANNUAL REPORT
The 2020 MSA Annual Report is available in the “About” section of MSA’s website: www.minsocam.org. The report provides highlights of MSA’s programs, publications, communications, events, and governance during the past pandemic year. You will find features on the 2020 awardees (Dr. Andrew Putnis, Roebling Medal; Dr. Daniela Ruhatto, Dana Medal; and Dr. Jin Liu, MSA Award); student research grant winners (Hannah Tompkins, Behnaz Hosseini, and Md Abu Raihan Chowdhury); publication statistics; Minerals Day events; communication outlets; education and outreach programs; benefactors; and much more.

THE 2021 CALENDAR

AWARD NOMINATIONS
Nominations are sought for the 2022–2023 awards.

The Roebling Medal (2022) is MSA’s highest award and is given for eminence as represented by outstanding published original research in mineralogy.

The Dana Medal (2022) recognizes continued outstanding scientific contributions through original research in the mineralogical sciences by an individual in the midst of his or her career.

The Mineralogical Society of America Award (2022) is giving for outstanding published contribution(s) prior to the nominee’s 35th birthday or within seven years of their PhD.

The Distinguished Public Service Medal (2023) is presented to an individual who has provided outstanding contributions to public policy and awareness about mineralogical topics through science.

Society Fellowship is the recognition of a members’ significant scientific contributions. Nomination is undertaken by one member, with two members acting as cosponsors. A form is required. Please contact the committee chair or the MSA home page.

Submission requirements and procedures are on MSA’s home page: http://www.minsocam.org/.

Mark Ghiorso in New Zealand

PRESIDENT’S LETTER

Why be a Member of the MSA?
I write this, my fourth President’s Letter, in mid-April 2021. Things are looking up, at least in the US, regarding the pandemic. The federal government once again respects science and makes policy decisions accordingly; vaccinations are becoming available and, at least where I live, there is little hesitation in taking advantage of that availability. Of course, things are not yet back to “normal.” Meetings are still being morphed into virtual extravaganzas and there are advantages to that format. There are also disadvantages. Attendees listen to talks more, as the option of milling around and talking about hiking, where to eat and what to drink, has all but vanished. However, the positive social and research consequences of milling about—new collaborations, a discovery of common interests, and all the other serendipitous aspects of social interaction—are gone. Of necessity, research presentations are recorded, often prerecorded, and are available to watch at one’s leisure. No more rushing from room to room hoping to catch a talk only to discover that the Chair has lost control of the schedule and thrown everything into disarray. These alternatively structured meetings are perhaps more civil and, arguably, more civilized. Is that a good thing? Will the research meeting of the future be forever changed and emerge as a hybrid of what necessity forced upon us? I suspect that it will, and I think that is a good thing, because it forces us all to reevaluate how we do business and whether the traditional practices are still the most effective way to best communicate our science.

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As always, stay safe and stay healthy,

Mark Ghiorso, 2021 MSA President
F. DONALD BLOSS PUBLICATIONS NOW IN DIGITAL FORMAT

Crystallography and Crystal Chemistry: An Introduction and Optical Crystallography are both now available as watermarked downloadable pdfs. Both classics in their field and still in use after many years, these publications can be ordered through MinPubs.org.

DID YOU KNOW?

- The American Mineralogist has been published from 1916 to the present day. All issues from 1916 through 1999 are available on MSA’s website through the link “Online Access” to American Mineralogist.
- The images, animations, and videos that are part of the Mineralogy & Optical Mineralogy textbook (Dyar, Gunter, and Tasa, 2020) are on the MSA website under the “Publications/Textbook” pulldown menu. The full-color graphics are organized chapter-by-chapter and are easily identifiable through thumbnail illustrations on the website.

The 2020 International Mineralogical Association (IMA) Council Meeting and IMA Business Meeting were initially scheduled to take place during Fall 2020, during the 3rd European Mineralogical Conference (emc2020) in Kraków (Poland). However, the conference was postponed until August 2021 (https://emc2020.ptmin.eu) because of the global pandemic, and it was decided that the needs of our association and its membership would be best served by conducting the council and business meetings online – in the best traditions of our time! Between January 11th and 14th, members of the IMA Council met with one another and with national representatives from across 17 time zones to discuss the future of our association, the achievements of its committees and commissions, changes to the council membership, upcoming IMA meetings, and other timely topics. While we all would have preferred to interact in person (perhaps over a glass of Kraków nalewka), and some of us may not have been fully awake at 6 a.m. or it was well past our bedtime at 1 a.m., the meetings were a great success.
At the time of writing, some of us are entering our fourth “wave” of Covid-19 infections. We hope that this one won’t be accompanied by the extreme loss of life that was characteristic of previous waves. I have wondered when will it be a good time to review the status of the MinSoc post-COVID-19? Will there really be a time when we can say that we are “post-COVID”? With that in mind, let’s have an interim review of our status. What have we lost? What have we gained? What have we learned?

On the debit side ...

- In-person meetings feel like a distant memory. My colleagues live inside my computer screen. No chats. No friendly cups of coffee during conference sessions.
- Researchers, in many cases, can’t go to the laboratory or into the field. Students on tight deadlines can’t get the research done that they need for thesis purposes. And students can’t go to a physical classroom to be with their lecturers.
- No data means no papers, right? Maybe.
- Grants to students have been limited by the restrictions on travel (both national and international).
- The awards that we give to shining lights in our scientific community have not been able to take place in the usual way.

So, not great really.

On the credit side, however ...

- We changed in-person meetings to virtual meetings. We still had great science, we had larger audiences than usual, and people who could not normally attend meetings found that they could. The Metamorphic Studies Group meeting in June 2021 was attended by people from 38 countries!
- Our journals have continued to flourish through the pandemic. We have ample content. In fact, submission numbers actually increased throughout 2020 and 2021. And both journals achieved improved impact factors, which were announced end-June 2021: Mineralogical Magazine attained 2.06 and Clay Minerals attained 1.48.
- Payments through our student grants system have been reduced but we have covered costs for attending virtual meetings. Our Mineral Physics Group created a “hardship” fund and used its funds to support some needy students. Normal service will resume in due course.
- We have selected awardees for all of our medals throughout the pandemic. Under normal circumstances, we present medals in person, and with some fanfare. Medals arriving as a small package in the post do not have quite the same impact! However, we now have plans to hold online seminars, where medallists can present their work, and where we can have an awards ceremony of sorts. This is not as good as being there in person and offering personal congratulations, but it does mean that we get to say lots of nice things about these deserving people to an appreciative audience. This seminar series will commence at the start of the academic year, so keep an eye on the Mineralogical Society website.

The Student Award scheme is being run as normal. The best student from each relevant Earth science/geology/mineralogy department receives a prize from the MinSoc (and two years membership). Any bonuses? Yes, a number.

1. Wherever possible, going forward, we will hold hybrid meetings (suitable for both in-person and virtual attendance). This will mean that attendance will be possible for all. Care will be needed that this new offering doesn’t break the financial model. Conference fees still need to cover the cost of hiring physical spaces, abstract volumes, etc. But we plan to make attendance free to people from Research4Life countries.

2. The MinSoc has not been alone in responding to equality, diversity, inclusivity (EDI) questions posed over the past 18 months. Staff, council members, society leaders, and others have all played important roles in thinking through our future role in EDI. We have recently finished our international survey of members and non-members, and there will be a report by the end of the year. It is clear that there are changes afoot to the ways in which we carry out most society activities. And we want all society members to come on board. Non-members who wish to join our activities will agree to abide by our Code of Conduct and other EDI legislation to be decided.

3. The society is rewriting its bye-laws. Hardly the world’s most exciting task, but this is not just a so-called “root and branch” review: we’re digging up the entire garden and replanting. We’re going as far as revising our mission statement – the very definition of why we exist. Opportunities for work like this do not come along very often and it is timely, given EDI considerations. It is also an opportunity to revise how our Special Interest Groups operate. Changes allowed by the new bye-laws will make for more dynamic, inclusive, and active groups. Remember that Special Interest Groups are only as productive as the people who lead them, so please consider offering your services to one (or more). Extra assistance is always welcome.

4. We have run two very successful webinar series, that of the Geomicrobiology Network and that of the Applied Mineralogy Group. Videos of almost all of these presentations are available now on Youtube through the society’s website.

5. We have done considerable work developing our Youtube Channel and now have ~100 presentations available for download. View content and subscribe at https://www.youtube.com/channel/UCJLevvFJEAtt2SRHozqd7LQ/videos.

6. Stocks of all of our medals expired last year. We took the opportunity, when moving to a new supplier, to refresh the design for two of them. We look forward to awarding these to deserving scientists.

7. The Hazel Prichard Bursary ran as normal (though slightly delayed) in 2021. The three joint winners for this year are as follows: Alexander Taylor Kong, Eliot Jones, and Ethan Shaw, all of whom have been MSc students in mining geology at the Camborne School of Mines (University of Exeter, UK). Their three-pronged project was based on the Ben Buie Complex (Isle of Mull, Scotland) and had the aim of providing a greater understanding of magmatic differentiation and layering processes within the British Palaeogene Igneous Province, identifying key controls on the potential for Ni–Cu–Co–PGE and V–Ti(Fe) mineralisation within the region. The students investigated the geometry of the intrusion and the controls on mineralisation in this layered mafic–ultramafic complex.
8. We continue to work on our outreach plans. This is gaining momentum, with James Byrne, the MinSoc’s new Public Relations Officer, leading representatives from the Special Interest Groups in deciding how best to achieve this.

So, all in all, a reasonably satisfactory state of affairs. We look forward to a return to more “normal” (I’m beginning to hate that word) activities, but also to bringing with us those new tricks that we’ve learned during the adverse, Covid-19 conditions.

Kevin Murphy, Executive Director

GEOMICROBIOLOGY NETWORK RESEARCH IN PROGRESS MEETING

Date: 15–16 September 2021

Venue: This year’s Research in Progress meeting will be held virtually via Zoom. We will use Gather.Town for our poster session.

Speakers will include: Arwyn Edwards, Kenda Lynch, Jon Lloyd and Ana Santos.

The abstract deadline is 1 September 2021; the registration deadline is 10 September 2021.

There is no charge to attend, but registration is required at https://www.minersoc.org/geomicrobiology-network-rip-2021.html

NEW TOPICS IN MINERALOGY 2: THE MINERAL–MICROBE INTERFACE THROUGH TIME AND SPACE

2–3 December 2021
Burlington House, London

The Mineralogical Society is delighted to announce a two-day New Topics in Mineral Sciences meeting that will focus on the importance of the mineral–microbe interface. Topics explored will be diverse and include the role of mineral surfaces in the emergence of life on Earth (and potentially other planets), and the key role that this mineral–microbe interface plays in controlling modern global biogeochemical cycles. Recent advances in the fundamental understanding of these important processes will be presented, alongside more applied aspects of the mineral–microbe interface. The latter will include the new biotechnological innovations that underpin sustainable mineral bioprocesing, biomineratisation, bioremediation and energy applications. We are planning a hybrid meeting, with presentations from international leaders in the field, alongside contributions from early career researchers working across the “geo” and “bio” disciplines.

At the time of writing, we are hoping that an in-person, hybrid, event at Burlington House will be possible. Status updates are expected throughout the remainder of the summer. If we must, we will switch to an all-virtual presentation, but for now we’re hoping to see some fellow scientists for real!

MEETING REPORTS

Metamorphic Studies Group 40th Anniversary

A report of this meeting is available at https://www.minersoc.org/msg-rip-2021.html and a montage of the people involved in the group (some since its foundation) has been created by current chair, Catherine Mottram. An enlarged version is available on the website.

Clay Minerals Group—Environmental Mineralogy Group Joint Annual Meeting

There was also the joint meeting “Minerals in the Natural and Built Environment” from the Environmental Mineralogy Group and the Clay Minerals Group.

This one-day meeting included the keynote presentation by Prof. Karen Hudson-Edwards (University of Exeter, UK) entitled “Minerals in Contaminated Environments: >25 Years of Research, Reflection and New Ideas”, and the annual George Brown Lecture, this year given by Prof. David Manning (Newcastle University, UK) and entitled “Mineral Stabilities in Soils: How Minerals can Feed the World and Mitigate Climate Change”. Recordings of these talks are available from the Meeting Report section of the MinSoc’s website.

Prizes were awarded as follows:

Environmental Mineralogy Group
- Best Oral Presentation: Callum Robinson (University of Manchester)
- Best Poster Presentation: Jody Grassby (University of Exeter)

Clay Minerals Group
- Best Oral Presentation: Harry Brooksbank (Newcastle University)
- Best Poster Presentation: Maggie White (Newcastle University)
**Meteoritical Society**

**http://meteoricalsociety.org**

**REPORT OF THE METEORITE NOMENCLATURE COMMITTEE**

The classification and reporting of new meteorites to the Nomenclature Committee (NomCom) of the Meteoritical Society (MetSoc) has continued throughout this pandemic year. We have passed 65,000 approved meteorites in the database, some 12,000 having a classification description and which includes over 430 lunar and 290 martian meteorites. I would like to thank all the NomCom members and all the finders and classifiers for their continuous effort to safeguard proper documentation for the naming, classification, and correct repository of specimens. Special acknowledgements go to outgoing members Emma Bullock (Carnegie Institution of Washington, USA), Hasnaa Chennaoui Aoudjehane (Université Hassan II de Casablanca, Morocco), Vincenzo Debaillé (Université Libre de Bruxelles, Belgium), and Brigitte Zanda (Muséum national d’Histoire naturelle Paris, France) who finished their terms. We welcomed four new members last January: Cyrena Goodrich (Lunar and Planetary Institute, Texas, USA), Ansar Greshake (Museum für Naturkunde Berlin, Germany), Juliane Gross (Rutgers University, New Jersey, USA), and Nancy Chabot (MetSoc Vice President; Johns Hopkins University Applied Physics Laboratory, Maryland, USA).

NomCom is currently composed of nine appointed members: Audrey Bouvier (Chair; Universität Bayreuth, Germany), Massimo D’Orazio (Università di Pisa, Italy), Cyrena Goodrich, Ansar Greshake, Juliane Gross, Mutsumi Komatsu (Sokendai, Japan), Francis McCubbin (Deputy Editor; NASA Johnson Space Center, Texas, USA), Bengkui Miao (Guilin University of Technology, China), and Devin Schrader (Arizona State University, USA). There are also three ex-officio NomCom members: Jérôme Gattacceca (Meteoritical Bulletin Editor; CEREGE, Aix-en-Provence, France), Jeff Grossman (Database Editor; NASA Headquarters, Maryland, USA), and Nancy Chabot (MetSoc Vice President; Johns Hopkins University Applied Physics Laboratory, Maryland, USA).

The purpose of the Nomenclature Committee is to approve new meteorite names and to establish guidelines and make decisions regarding the naming and classification of meteorites. New meteorites, dense collection areas, type-specimen repository collections, and revisions are published through the Meteoritical Bulletin and the Meteoritical Bulletin Database (MBDB) (https://www.lpi.usra.edu/meteor/).

**Meteorites:** The 2019 entries of the MBDB, which totals 2,141 meteorites, have been published by Gattacceca et al. (2020) in issue 108 of the Meteoritical Bulletin (MB). The full write ups of 1,394 non-Antarctic meteorites and supplementary tables can be found online as supporting information and in the MBDB Archive. The MB issue 108 includes 12 approved falls, including four more for 2018: Benenitra (L6, Madagascar, 27 July), Komaki (L6, Japan, 26 September), Ksar El Goraaine (H5, Morocco, 28 October), Mhabes el Hamra (H4/S, Mauritania, 23 December) and four for 2019 with Aguas Zarcas (CM2, Costa Rica, 23 April), Oued Sfayat (H5, Algeria, 16 May), Taaqtaq-e Rassoul (H5, Iran, 10 August), and Víñales (L6, Cuba, 1 February).

**Meteoritical Bulletin** issue 109, which will contain meteorites approved in 2020, is in preparation. It will contain 2,790 meteorites, including 1,249 non-Antarctic meteorites and a remarkable 17 falls. These are 4 more for 2019 Al Farcia (L6, Western Sahara, 20 August), Flensburg (Cl-ungrouped, Germany, 12 September), Mahadeva (H5, India, 22 July), and Wad Lahbeyya (H5, Morocco/Western Sahara, 27 June); and 8 so far reported for 2020: Cavezzo (LS-an, Italy, 1 January), Gatuto (L6, Kenya, 24 April), Kolang (CM1/2, Indonesia, 1 August), Narashino (H5, Japan, 2 July), Novo Mesto (L5, Slovenia, 28 February), Santa Filomena (H5-6, Brazil, 19 August), Tarda (C2-ungrouped, Morocco, 25 August), Tiros (Eucrite, Brazil, 8 May), and Zhob (H3-4, Pakistan, 9 January).

**Dense Collection Areas:** There are currently over 370 collection areas named as dense collection areas (DCAs).

Twenty-one new DCAs were defined last year in Algeria (Hassi el Biod Algeria, Hassi el Madani, Raïfa, Tibetatâine); Chile (Toconao); China (Pakepake, Tazhong, Kuiyibage, Liuyuan); Iran; Libya (Gadamis, Ghadduwaq, Oiuru); Mali (Tisserlit-line); Mauritania (El Hassan Ould Hamed); Morocco (Akka, Tata, Tazzarine); Niger (Gouchi); and United States (Black Butte Nevada, Crescent Valley).

**Type-Specimen Repositories:** Five new type-specimen repositories were approved:

AuckMus – Auckland War Memorial Museum (New Zealand); IST-USTHB – Université des Sciences et de la Technologie H. Boumediene, Algiers (Algeria); Ubayr – Bayerisches Geoinstitut, University of Bayreuth (Germany); Ugöt – Georg-August-Universität Göttingen (Germany); and UOslo – Natural History Museum University of Oslo (Norway).

**Meteorite naming:** Remember to send your write-ups for new and provisional names to the NomCom at least three weeks before submitting your conference abstract or manuscript to journals to avoid potential issues with naming and classification and delays in publication. The release of the write-up to the database may be held on request if there is an embargo from publishers.

**Useful database tools:** Meteorites and associated open source data of the MBDB can be searched by various categories including oxygen isotopes. Once a search is made, a weblink is created at the bottom of the search page and can be imported into a data spreadsheet software program to create tabulated data.

Finally, please do not hesitate to contact us with questions or concerns about the NomCom, especially with suggestions for improvement.

Audrey Bouvier  
Chair of the Nomenclature Committee  
Universität Bayreuth

**GIFTS AND GRANTS GUIDELINES**

The stated mission of the Meteoritical Society is “to promote research and education in planetary science with emphasis on studies of meteorites and other extraterrestrial materials that further our understanding of the origin and history of the solar system.” Besides the society’s publications, the annual scientific meetings, establishing official names for newly found meteorites, and the awards sponsored by the society, there are other ways by which we work toward furthering our mission. This includes supporting student travel to conferences and workshops; supporting student research; assisting scientists from economically disadvantaged countries; supporting classes or field schools, especially those that bring meteoritics and planetary science to developing countries; compiling oral histories from prominent members of the society; and supporting outreach to the broader public community on meteoritics and planetary science.

To support these activities, the society has created the Endowment Fund. The majority of the endowment consists of the General Fund, which can support one-time activities that are not part of the normal society business. The Endowment Fund also has named funds: the
Nier Fund, the McKay Fund, and the Travel for International Members Fund, all of which were established for the specific purposes described in the following section. Details about activities supported by all of these funds are given under the “Activities Supported” section of the society’s website.

For those who wish to assist in this mission, donations can be made to the General Fund or to any of the specific funds (see “Ways to Contribute” on the society website).

**ANNUAL MEETING SCHEDULE**

<table>
<thead>
<tr>
<th>Year</th>
<th>Location</th>
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<tr>
<td>2021</td>
<td>Chicago (Illinois, USA)</td>
<td>15–20 August</td>
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<tr>
<td>2022</td>
<td>Glasgow (Scotland, UK)</td>
<td>14–19 August</td>
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<td>2023</td>
<td>Perth (Western Australia)</td>
<td>2–7 July</td>
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<td>2024</td>
<td>Brussels (Belgium)</td>
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**RENEW YOUR MEMBERSHIP NOW!**

Please don’t forget to renew your membership for 2021. Students: this is particularly important if you are interested in applying for one of our student presentation awards, as you must be a member to be eligible. You can renew online at: https://meteoritical.org/membership/join

In 1989, Longman published a seminal book by Bruce Yardley entitled *An Introduction to Metamorphic Petrology*. Clearly written and well-illustrated, this was a much-needed textbook. I will not have been the only academic who built lecture courses around it and put it on the “must buy” list for libraries and students. Just over 30 years later and a second edition has arrived, published by Cambridge University Press and with Clare Warren (Professor of Metamorphic Petrology at the Open University, UK) as a co-author.

In those 30 years, the science of metamorphic petrology has seen significant steps forward. Leaps forward in microbeam technology have enabled better imaging, mapping, and microanalysis. But there have been two key game changers: first, thermodynamic modelling incorporating not only $P$–$T$ calculations but also pseudo-section analysis; second, the increased precision of isotopic dating that enables precise calculations of $P$–$T$–$t$ paths. This is what Professor Mike Brown (University of Maryland, USA) has referred to as a “Golden Age of metamorphic petrology”.

In their preface, Yardley and Warren say that this “is a completely new edition” designed as a “core textbook for second and third year undergraduate metamorphic petrology courses and to support more-advanced teaching”. Although this is true, the structure of the book is, at heart, little changed. Chapters entitled “The Concept of Metamorphism”, “Metamorphism of Pelitic Rocks”, “Metamorphism of Basic Igneous Rocks” and “Metamorphism of Calc-Silicate Rocks” are all there, although greatly updated. Other chapters have been split into two, and there is a new chapter entitled, “The Duration of Metamorphism”.

The early chapters are built around the importance of attaining chemical equilibrium in determining metamorphic assemblages. The later chapters integrate this with the role of deformation and overall tectonic processes. Although not much is made here of pseudo-sections or of the thermodynamics that supports them, these chapters are underpinned by the advances in technology which can link $P$–$T$–$t$ paths to deformation histories. Chapters 9 (“The Duration of Metamorphism”) and 10 (“Metamorphism and Tectonics”) both utilise key examples and are excellent syntheses of the current state-of-the-art. A key question might be this: Is this book built around description of fact or around processes? That the two overlap is implicitly obvious in understanding metamorphism. I think that this book leans towards the former, which is not necessarily a bad thing.

Many of the diagrams from the original edition are included, although most are redrawn and in colour. There is also a welcome increase in the number of field images and petrographic images that are in colour. The only issue that I have is that a lot of these images are too small. This is clearly an editorial decision, but I do wonder whether increasing the size of many of these images (albeit at the expense of increasing the number of pages) would have been worthwhile. Although there are more pages in this book than in the first edition, I doubt if the word count is any greater because the font size is much larger. The font size and layout make this a very pleasant book to read. It is easy on the eye.

The first edition of this book was excellent. This second edition is a great successor and it comes with a Cambridge University Press hosted webpage which contains supplementary material. I have no hesitation in recommending this excellent book to any academic who is teaching a metamorphic petrology course or to any student wishing to follow a route into metamorphic petrology.

*Peter J. Treloar*

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Silicon carbide (SiC) minerals, which were argued to condense in stellar winds, were first isolated and imaged in 1987 (Bernatowicz et al. 1987). However, their existence in meteorites had been speculated from extensive noble gas studies. These studies suggested that SiC minerals are the carrier phases of the exotic $^{128,130}$Xe and $^{22}$Ne isotopic anomalies that can be found in primitive meteorites (e.g., Anders and Zinner 1993). In fact, SiC stardust does carry large isotopic anomalies, up to 4 orders of magnitude, both in light mass elements (e.g., carbon, nitrogen) and in medium mass elements (e.g., magnesium, iron, titanium). These anomalies can only be produced in stars through nuclear reactions occurring at extreme temperatures, by which the structure of the atomic nucleus is altered. The extreme isotopic anomalies in the SiC dust grains were not completely homogenized during the first 10 million years of planet formation and Solar System evolution, so they have kept their compositions intact until today. The dust grains carrying these enormous anomalies can be identified in extraterrestrial rocks that fall to Earth.

Not all meteorites contain stellar dust grains. They are only present in the fine-grained matrix in primitive chondrite meteorites, which are rich in carbon and other organic materials. This is why samples from carbonaceous type (C-type) asteroids Bennu and Ryugu, subjects of ongoing missions, are such an exciting prospect. The abundance of stardust in meteorites is a function of the temperature and fluid–rock reactions occurring in the interiors of stars, alteration in the interstellar medium, and aqueous and thermal processes on asteroid bodies. One such stellar source of dust grains is Type II core-collapse supernova explosions that occur when a $>8$ solar-mass star explodes after having already formed oxygen, magnesium, silicon, sulfur, argon, and calcium in the neon- and oxygen-burning zones of the star’s interior. Once the star fuses silicon to form an iron core, energy production halts because iron has the largest nuclear binding energy per nucleon. Because the pressure from the overlying gas is no longer balanced by fusion in the core, implosion of the central core occurs and raises the core temperature to $5$ billion Kelvin. Photons emitted from the core dissociate the iron atoms, which break apart into helium nuclei and allow for the compression and formation of a nucleon gas and the formation of a proto-neutron star that can resist the gravitational collapse. As the proto-neutron star halts the core collapse, it recoils. This release of gravitational potential energy generates a shockwave that ejects the remaining stellar material and leaves behind a neutron star. When the shock wave collides with the inner layers, it ejects matter outwards at $\sim 10,000$ kilometers per second. This is known as the core bounce. This shock wave is quickly stalled because energy is lost, but it gets reheated by the capture of energetic neutrinos near the proto-neutron star. Ejection of these neutrinos rapidly drains energy from the core. Once core bounce has occurred, further neutrino emission takes place in the proto-neutron star, and it is this neutrino-heating mechanism that revives the stalled shock front. The core-emitted neutrinos contain $\sim 10^{54}$ J of energy. About 1% of these neutrinos are captured by material within the stalled shock wave. The shock heats material as it travels outward, resulting in explosive nuclear burning that produces abundant amounts of $^{13}$C, $^{15}$N, $^{26}$Al, and $^{44,47,49}$Ti isotope species (Fig. 1). The seed nuclei can be heated to temperatures of several $10^{10}$ K within the hearts of core-collapse supernova explosions, also leading to exotic iron-group elements.

It is from the resulting ejecta of a core-collapse supernova that a fraction of the stellar dust—now present in the Solar System—condensed. These dust grains show extremely large enrichments in the isotopes $^{13}$C, $^{15}$N, $^{26}$Al, and $^{28}$Si, the origins of which have long been proposed to be classical novae (Amari et al. 2001). Less energetic classical nova outbursts occur in close binary systems containing a carbon–oxygen or oxygen–neon white dwarf and a Sun-like companion. Bose and Starrfield (2019) had discussed this possibility by imposing different mixing conditions on novel carbon–oxygen nova models and comparing their isotope yields to SiC stardust. They showed that the best solutions were achieved when there was a mixing of material after thermonuclear runaway had occurred. However, the compositions of the dust in classical nova

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**FIGURE 1** The formation and location of a revived shock wave due to enhanced neutrino production in a supernova explosion results in abundant $^{13}$C, $^{15}$N, $^{26}$Al and several Ti isotope species. The red region is heated while the blue region is cooled by neutrino production and transport. The SiC D grains form in winds consisting of the innermost ejecta in a 15 solar-mass core-collapse supernova. The SiC grain secondary electron image is from Zinner (2014).
outbursts are more extreme than those observed in stardust grains (Fig. 2). Possible origins for selected grains in core collapse supernovae was discussed because of the existence of both proton- and neutron-capture isotopic signatures in 1-D models, indicating heterogeneous hydrogen ingestion into the He shell in pre-supernova stars (Liu et al. 2016). Schulte et al. (2021) compared the isotopic compositions of these rare stardust grains to new 3-D core-collapse supernova simulations created by Patrick Young of Arizona State University (Fig. 2). They found that the abundant isotopes ($^{12}$C/$^{13}$C < 20 and $^{14}$N/$^{15}$N < 60) in these rare stardust grains, which they have renamed “SiC D grains”, are produced deep within the core-collapse supernova and, thus, that SiC D grains could form from winds consisting of the innermost ejecta from a 15 solar-mass core-collapse supernova (Fig. 3). Furthermore, they found that the source material for SiC D grains is enriched in the important short-lived radionuclides $^{26}$Al and $^{44}$Ti, the progenitors of $^{26}$Mg and $^{44}$Ca, which have been carefully studied in the fields of astronomy and planetary science. This SiC stardust will form in the ejecta shortly after being accelerated by the shock wave and subsequently injected into the protosolar nebula. These grains can then survive in the primitive carbonaceous chondrite parent bodies that form early in the Solar System’s history, some of which find themselves captured by Earth to become meteorites.

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PHASE EQUILIBRIUM MODELLING: APPROACHES AND PITFALLS
REPORT ON THE ON-LINE WORKSHOP

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The no-cost, online phase equilibrium modelling workshop entitled Phase Equilibrium Modelling: Approaches and Pitfalls was held 10–14 May 2021. The workshop was organised and presented by Dave Pattison and Jacob Forshaw (both from the University of Calgary, Canada), Pierre Lanari (University of Bern, Switzerland), Dave Waters (University of Oxford, UK), Mark Caddick (Virginia Tech, USA) and Doug Tinkham (Laurentian University, Canada) (Fig. 1). The meeting was jointly sponsored by the Mineralogical Association of Canada, the Mineralogical Society of Great Britain and Ireland, the Mineralogical Society of America, and the Société Française de Minéralogie et de Cristallographie. A total of 638 scientists from 47 countries registered for the online workshop, compared with 35 registrants for the equivalent COVID-cancelled in-person workshop at the May 2020 Geoconvention meeting in Calgary.

The rationale for the workshop was that all practicing and up-and-coming metamorphic geoscientists should have a nuanced understanding of the potential, but also the pitfalls, of phase equilibrium modelling. The first two days of the workshop focused on thermodynamic databases and three of the most commonly used metamorphic phase equilibrium modelling software packages: THERMOCALC, Perple_X, and Theriak-Domino. Days three and four focused on factors that influence the interpretation of a phase equilibrium model, including uncertainties in phase equilibrium modelling, reactive bulk composition, the interplay between equilibrium kinetics in petrological interpretation, and an assessment of predicted phase equilibria versus natural constraints. Day five consisted of shorter presentations that addressed topics requested by the registrants.

The workshop was conducted by Zoom webinar and hosted by the Faculty of Science at the University of Calgary. The workshop ran for 3.5 hours each day for the five consecutive days. The first four days featured two 45–60 minute lectures, each followed by a dedicated question-and-answer (Q&A) session, with a 15 minute break between. A 30 minute open Q&A session concluded each day. Registrants submitted questions to a moderator who posed those questions to the presenters. The presentations and the Q&A sessions on day five were shorter and less structured.

The lectures and associated Q&A sessions were recorded. These, along with pdf documents of the presentations, are available for public access and to download from the workshop’s website: http://e-thermo-workshop-2021.petrochronology.org/. These materials are, or will be, available on the websites of the Mineralogical Association of Canada, Mineralogical Society of Great Britain and Ireland, the Société Française de Minéralogie et de Cristallographie, and the Mineralogical Society of America.

The large registration was unexpected and encouraging. Of note was the high number of students and post-doctoral fellows (combined, about 70% of the registrants), and the 39:61 ratio of female to male registrants (Fig. 2A). The majority of registrants described themselves as novice or intermediate in terms of their experience with phase equilibrium modelling (Fig. 2B). Of those who had used the different software packages there was a fairly even distribution, with use of Perple_X being slightly higher than the other two (Fig. 2C).

**Figure 1** Title slide of the on-line workshop Phase Equilibrium Modelling: Approaches and Pitfalls, which was held 10–14 May 2021.

**Figure 2** Registrant profile and satisfaction of the on-line workshop Phase Equilibrium Modelling: Approaches and Pitfalls.
Reaction to the workshop, based on 206 responses to the post-workshop survey, was positive. Over 97% of attendees said that the workshop was helpful, that they would attend again, and that they would recommend it to others. The most positive reaction to the workshop came from those of intermediate and, especially, novice experience (Fig. 2D), and from the 71% of registrants who attended all five days of the workshop. More than 97% agreed or strongly agreed that the webinar format was effective and that the content was appropriate, and 96% agreed or strongly agreed that the workshop encouraged them to do phase equilibrium modelling. Whilst several respondents remained loyal to the software they had previously used, many expressed interest in trying out other software packages. The three most commonly cited criticisms of the workshop—especially from those with no prior experience of phase equilibrium modelling—were, 1) a desire for more hands-on tutorials and exercises for the different software packages, 2) a desire for more case studies and specific applications, and 3) the fact that there was a lot to digest each day.

Some of the most commonly cited “take-aways” from the workshop included the following: appreciation of the differences between the software packages; the importance of choice of thermodynamic database and solution models for a given phase equilibrium model; the importance of assessing the reactive bulk composition for a successful model; the type and magnitude of uncertainties on calculated phase equilibria; and the way in which metamorphism is an interplay between equilibrium and kinetics. However, the two biggest ones were that A) the rocks are always right (that is, models are not reality, they are just models); and B) the fact that phase equilibrium modelling is not a “routine” endeavour: it offers great potential while demanding careful thought and analysis.

One aspect of the workshop that was of more than petrological interest was the vast reach of the workshop compared to its in-person precursor (638 vs. 35 registrants). The change to an online format was catalysed by the COVID-19 pandemic, yet the implications of this change go beyond the pandemic. Many registrants had neither the time nor the money to attend the originally planned in-person event yet were able to attend and benefit from the online event. Some noted that an online event can’t replicate the depth of interaction of an in-person event—a view we don’t dispute—but that this was counterbalanced by the increased reach of the online event. Perhaps a blend of online and in-person events (such as workshops or scientific meetings) will be the way of the future.

Submitted on behalf of the organisers:
Dave Pattison, Jacob Forshaw, Pierre Lanari, Doug Tinkham, Dave Waters, and Mark Caddick

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**Critical minerals: From discovery to supply chain**

**Online workshop November 16-18**

This online workshop will address the critical minerals needed to grow low-carbon economies, emphasizing those used in battery, magnet, and photovoltaic technologies.

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**Program**

http://cmscontent.nrs.gov.bc.ca/geoscience/content/2021_CriticalMineralsWorkshop_PreliminaryProgram.pdf
International response to COVID-19 has resulted in scientific meetings being canceled or postponed. Check meeting web pages for ongoing updates.
The Oxford English Dictionary defines ‘vector’ as a quantity having direction as well as magnitude, and ‘scalar’ as a quantity having only magnitude, not direction. Much geological research starts with fieldwork, manifestly a vector activity. In Figure 1A, the geologists are exploring the intersection of a complex, 3-D body, the layered Klokken syenite, a 4 × 3 km igneous intrusion in the Gardar alkaline province of SW Greenland, with a mountainous 3-D land-surface. I described the unusual layering in Elements v10n1 (Parsons 2014). The igneous rocks were emplaced 1,166.3 ± 1.2 million years ago, and the 650 m of 3-D topography, which reveals the inner workings of the magma chamber, was carved by the advance and retreat of the mighty Greenland ice sheet in the last few thousand years. Only the age (a U–Pb age from baddelyte, ZrO₂) is a scalar quantity.

Klokken is in the Gardar Rift, famous in petrological circles because of the absence of disturbance, physical or chemical, of its ancient, mineralogically complex alkaline rocks since their emplacement. The rift includes a 1,200 m thick sequence of unmetamorphosed red sandstones. The U–Pb age was obtained as part of a NASA-sponsored project to investigate whether isotopic decay constants change over time. Based on this high-precision age, mica from a late member of the intrusion has subsequently been used to recalibrate the 40K/39Rb decay constant employed today in Rb–Sr dating.

We use combinations of vector and scalar observations routinely in geology, but the vector–scalar interface is often more complex than appears at first sight. It has led us down some blind alleys and, sometimes, into protracted controversies. For me, personally, one of the interfaces involved so-called ‘multiple diffusion domain (MDD) noble gas thermochronology’, a method described recently in Elements by Gautheron and Zeitler (2020). With MDD, apparent ages obtained from the radioactive decay of 40K to 40Ar over time, a technique known as 40Ar/39Ar dating, and an Ar-release spectrum obtained during laboratory heating, are used to calculate the thermal history of rock samples over geological time, mostly using alkali feldspar, (Na,K)AlSi₃O₈.

When the method was first applied it was found that apparent ages obtained from alkali feldspars were often considerably younger than those obtained by other isotopic methods. Argon is an inert gas, and it was suggested, correctly, that leakage over geological time might be related to intergrowths known as ‘perthite’ which form when the alkali feldspar cools.

Perthite is composed of two intergrown feldspar phases, one Na-rich, the other K-rich (Figs. 1B–1D). It forms because of the large difference in ionic radii between Na⁺ and K⁺. The feldspar structure is based on a 3-D framework of Si–O and Al–O tetrahedra, with the alkali ions in the relatively large spaces between them. At high T, the Si–Al–O framework is flexible and can accommodate Na and K ions distributed randomly, but, as it stiffens during cooling, structural strain energy can be lowered only if they form clusters. The feldspar undergoes ‘exsolution’, forming ‘perthitic intergrowths’. The scalar world of isotopic ratios and the vector world of crystal microtextures become inextricably entwined.

In 1982, Bill Brown and I began using transmission electron microscopy (TEM) and scanning electron microscopy (SEM) to study the perthitic intergrowths in alkali feldspars in the Klokken layered series (Fig. 1A), to explore their evolution with respect to cooling rate, and to understand the role and mechanisms of fluid–feldspar reactions. Using TEM, we could image lattice nodes separated by only ~0.7 nm. From mountain-side to lattice: a vector scale range of 8 × 10¹¹.

The Klokken layered series is unique (Parsons and Becker 1987). The dark brown layers (Fig. 1A) are fine-grained syenites with a granular texture. Mineral chemistry shows that they are a roof-chill series which became detached from the roof of the magma chamber in sheets that sank like giant pizzas onto pale ‘laminated syenites’ accumulating by crystal settling below. Their brown surface was produced by recent periglacial weathering; underneath, the feldspar is dark green and glass-clear in thin section. The feldspars have very fine-scale perthitic intergrowths called ‘braid’ perthite (Fig. 1B), which coarsen systematically downward, with a near-perfect log–linear relationship between

### Figure 1

- (A) The summit ridge of the Klokken layered syenite intrusion. Scandinavian post-docs for scale. The dark brown layers are ‘granular’ syenites and the pale layers are ‘laminated’ syenites.
- (B) Transmission electron microscope image of a sub-optical coherent intergrowth in a feldspar from a granular syenite collected near the bottom of (A). Structural elements are arranged to minimize coherency strain energy. The stripy phase is Na-feldspar (albite). The stripes are twins on the Albite Law. The zig-zag phase is K-feldspar (microcline); each zig and each zag is a twin. This fully coherent microstructure has retained 94% of its radiogenic 40Ar since 1,166 Ma, giving it an apparent age of 1,096 Ma. (C) Backscattered electron image of a turbid alkali feldspar from a pale laminated syenite horizon in panel A. Dark areas are albite; light areas are microcline. The area near the centre is a braid intergrowth similar to that shown in (B). It is a relic of the microtexture prior to the deuteric coarsening that led to ‘patch’ perthite. The patches are individually a mosaic of subgrains (see D). Black dots are micropores, some containing a Mesoproterozoic fluid. This is a leaky feldspar. It has retained only 57% of its 40Ar, giving it an apparent age of 662 Ma. (D) Transmission electron microscope image of albite subgrains and micropores (irregular white areas) within an albite patch similar to the dark areas in (C). The tiny white dots are ‘burn holes’ along subgrain boundaries, produced during atom-milling.
their periodicity and topographic height. They are called ‘coherent’ intergrowths because lattice-scale TEM images show that the Si–Al–O framework remains continuous at the interfaces. The pale ‘cumulate’ layers (Fig. 1A) are produced by crystal settling. They are coarse-grained, have a pronounced lamination, or do not vary systematically in crystal size or mineral chemistry, and are mainly composed of white or grey turbid feldspars. The feldspars are mainly irregular ‘patch-perthites’ (Fig. 1C), formed by a dissolution–reprecipitation process called ‘deuteric coarsening’, driven by loss of coherency strain energy. The patches are composed of tiny ‘incoherent’ albite-rich or microcline-rich subgrains (Fig. 1D).

Turbidity is the norm in alkali feldspars in common plutonic rocks, such as granites. It is caused mainly by myriads of micrometre-scale, often fluid-filled, micro pores and by subgrain boundaries (Figs. 1C and 1D). In the Klokken laminated layers, hydrated mafic phases, such as amphibole and mica, appear, and the upward extensions at the top of some layers are pegmatitic. The laminated syenite layers clearly acted as high-T aquifers during the cooling of the pluton, while the fine-grained, granular syenite layers with glass-clear feldspars remained impermeable.

I stumbled into noble gas thermochronology because Klokken seemed to be the ideal place to investigate the role of perthitic intergrowths in the loss of radiogenic 40Ar. We (Parsons et al. 1988) found that coherent perthitic crystals (Fig. 1B) had retained almost all their 40Ar, giving nearly horizontal Ar release spectra of 1,162 ± 16 Ma and maximum ages on their nearly horizontal Ar release spectra of 1,162 ± 16 Ma. The least retentive incoherent patch perthites (Figs. 1C and 1D) had apparent ages as low as 662 Ma, and strongly stepped, inclined release spectra.

The feldspars had shared the same thermal history so the nature of the interfaces between Na-rich and K-rich regions of the perthite was clearly the factor controlling Ar loss since the Mesoproterozoic. Subsequent laser-probe work (Burgess et al. 1992) confirmed that the loss of 40Ar from regions of patch perthite could be accounted for by sustained heating of subgrains for 1,166 My in the upper crust at <150°C. All relevant microtextures formed within 0.1 My of the emplacement of the intrusion.

Multiple diffusion domain ‘thermochronology’ was introduced by Lovera et al. (1989) less than a year after Parsons et al. (1988) had appeared. Natural and laboratory Ar loss are modelled as a conceptual system of diffusion domains with simple shapes and a finite range of sizes and of Ar-loss pathways that release Ar instantaneously into a vacuum. The physical nature of the domains is inferred from the detail of the Ar release spectrum during step heating, during which the domains must remain unmodified. The domains are, effectively, scalar. Extraordinary claims for the MDD method have been made: for example, that the uplift history of Tibet can be calculated from a 40Ar/39Ar study of a single alkali feldspar sample (Richter et al. 1991). The contrast in approach to the vector, fieldwork, and microscopy-based paper of Parsons et al. (1988) could hardly be more striking.

The MDD picture of feldspar microtexture did not go down well with feldspar mineralogists and not with all Ar experts. Nevertheless, MDD modelling using feldspars became, and remains, widely applied. Joe Smith and Bill Brown, the leading experts on feldspars, sadly no longer with us, thought we needed to point out its deficiencies, which led to the appearance of Parsons et al. (1999). The snappy title is Joe’s. The publication of this paper was not straightforward, and carries an unsettling message. We submitted it to the journal that had published Parsons et al. (1988), but it was rejected on the advice of a single, anonymous, referee, who wrote:

‘In my view this is not science. The authors present a debating position paper on the value of the ‘multiple diffusion domain’ or MDD model for inverting Ar–Ar data to obtain cooling histories. There are 30 pages of text with one table and one schematic figure’.

There was no in-depth discussion of the shortcomings of the MDD method that had been systematically raised in the manuscript. I published my first paper in 1965 and this was my first and only outright rejection. I was UK editor of Contributions to Mineralogy and Petrology for 24 years. Every manuscript was reviewed by a minimum of two experts; more if they disagreed. I must have handled around 1,000 reviews. I saw none that rejected a paper in such a peremptory way. Most were kindly, thoughtful and helpful.

At a moment like this we need a philosopher, not a scientist. Here is what Karl Popper has to say on what science is and how it works (the italics are his):

‘Our theories, beginning with primitive myths and evolving into the theories of science, are indeed man-made, as Kant said ... We do try to impose them on the world, and we can always stick to them dogmatically if we wish, even if they are false. But although at first we have to stick with our theories—without theories we cannot even begin, for we have nothing else to go by—we can, in the course of time, adopt a more critical attitude towards them. We can try to replace them by something better if we have learned, with their help, where they let us down. Thus there may arise a scientific or critical phase of thinking, which is necessarily preceded by an uncritical phase’.

Karl Popper (From: Unended Quest: An Intellectual Autobiography, Fontana Paperbacks, 1976)

Science advances in an atmosphere of carefully reasoned criticism. It moves forward when we reject theories. The Sun does not circle Earth. Phlogiston does not exist. It takes only one black swan to falsify the statement ‘all swans are white’.

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