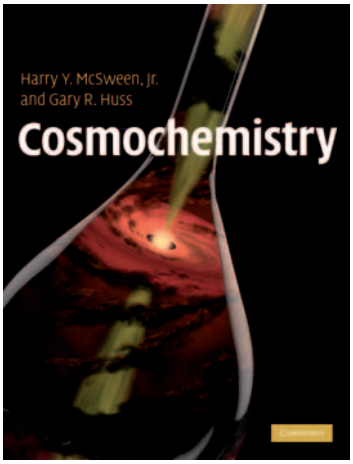
COSMOCHEMISTRY[1]

Cosmochemistry is an exciting, new and rapidly growing interdisciplinary field. A student of cosmochemistry is expected to have some knowledge of chemistry, physics, astronomy, mineralogy and geology. A scholarly presentation of all these aspects in a single publication has been lacking for many years. Charles Cowley's *Introduction to Cosmochemistry*, published in 2005, is too heavily biased towards astrophysics to qualify as a comprehensive cosmochemistry book. The new book by Hap McSween and Gary Huss entitled *Cosmochemistry* is to a large extent devoted to the chemical and isotopic composition of solar system materials, but it also contains sections on nucleosynthesis and solar physics and an appendix on analytical techniques. It provides an excellent introduction to the multidisciplinary field of cosmochemistry.

A comparison with Ross Taylor's *Solar System Evolution* (1992) reveals the enormous progress achieved during the last 18 years of cosmochemical research: (1) Advances in instrumentation for analyzing trace elements and stable and radioactive isotopes in meteorites and components of meteorites down to the micro- and nanometer scales have produced an incredibly precise chronology of the early solar system. (2) New dating tools, such as the ^{182}Hf–^{182}W system, have opened the way for the spectacular discovery that iron meteorites are older than stony meteorites. (3) Completely new types of meteorites have been identified. (4) A wealth of data from new missions to Mars, the Moon, the asteroids and comets has led to a quantum leap in our understanding of the formation and evolution of the solar system. All of this is competently and extensively reviewed in the McSween and Huss book.

The book begins with a definition of cosmochemistry as "the study of the chemical composition of the universe and the processes that produced these compositions." During the second half of the 20th century, cosmochemistry evolved as an offspring of geochemistry. Extraterrestrial materials were simply analyzed with instruments commonly used in geochemistry. This has completely changed. Following McSween and Huss, geochemistry may now be considered a branch of cosmochemistry. One can view cosmochemistry as the materials science of the universe. As McSween and Huss point out, the generally small size of valuable extraterrestrial materials has been and will be a driving force for improvement in analytical tools, which will provide collateral benefits to geochemistry, as exemplified, for example, in stable isotope cosmochemistry. Sophisticated procedures specifically developed for measuring tiny variations in stable isotopes among solar system materials find increasing applications in low-temperature geochemistry. Also, many of the isotope systems used for dating Earth rocks were first developed for the analysis of extraterrestrial samples and only later applied to the chronology of terrestrial samples. Examples include the Ar–Ar, Sm–Nd, Lu–Hf, and Re–Os systems.

Following the introduction, some basic nuclear physics and chemistry are presented, apparently addressed to a readership at the undergraduate level. With these tools at hand the origin of elements is discussed in some detail. This sequence highlights the procedure adopted by the authors for the entire book. Basic physics, chemistry and mineralogy are explained to the extent required for understanding the more complicated issues. A didactic approach is visible throughout the book. Each of the fourteen chapters is arranged in the same way, with an overview at the beginning and a summary after the main text; this is followed by a section with questions about the main message of the chapter and suggestions for further reading and references. The text is divided into many smaller units, sections and subsections with appropriate headings. I find this helpful as many readers will use the book mostly as a source of information on specific cosmochemical issues and problems.



Before discussing meteorites, the authors provide a detailed account of presolar grains; this excellent chapter is based on the extensive experience of the second author in this subject. In the following chapters, the authors stress processes of formation of meteorites and their parent bodies and avoid extensive discussions about naming and classifying meteorites and their components.

A full chapter is devoted to geochemical and cosmochemical fractionations – a very useful and informative section highlighting the similarities and differences of geochemical and cosmochemical processes. A first-order observation about the result of a typical cosmochemical process is the depletion of volatile elements in almost all solar system objects. In this and later sections, the authors emphasize evaporation of chondritic matter as their preferred model for producing the low volatile-element contents of most meteorites and planets. The authors consider the famous Ca–Al-rich inclusions (CAIs) as residues of episodic heating processes. Low temperatures prevailed throughout the formation of the solar system except for local heating events that produced chondrules. This point of view is not universally accepted. There is evidence in meteorites for condensation processes. Here the authors could have provided a more balanced discussion by mentioning alternative possibilities. Other chapters deal with chronometers and the chronology of the early solar system, and there is a chapter on highly volatile elements, mainly rare gases and organic matter.

The remainder of the book is devoted to the larger objects of the solar system: asteroids (as meteorite parent bodies), comets and the terrestrial planets. Included are discussions of the composition and evolution of the Earth, Mars, the Moon and Vesta. We have samples of all four of these. Early in their history they differentiated into a core, mantle and crust, but each of them has had a somewhat different evolution. Similarities and differences among the planets are subsumed in what is today called *comparative planetology*, a completely new area of research. The final chapter deals with the description of analytical tools and their applications, a worthwhile addition for scientists from other disciplines.

Despite the 550 pages of text, one will always miss one aspect or another, depending on one's personal preferences. I, for example, regret the absence of a presentation on recent modeling of the formation of the Earth and the other terrestrial planets, which has been done by Wetherill and later Stewart, Morbidelli and others. Impact enthusiasts will miss a section on impacts and terrestrial craters. It is, however, virtually impossible to cover all aspects of cosmochemistry in a single book.

The book is very well written. It goes into great detail when necessary and succeeds in explaining even complex facts with simple words, avoiding technical jargon. Most of the figures are excellent and focus on the main message. This is a style that the senior author has successfully applied in his earlier books on meteorites and the solar system. The book is complemented by tables with element abundances in some meteorites, condensation temperatures and other items.

In summary, *Cosmochemistry* gives a comprehensive survey of the present state of the science. I highly recommend it for undergraduate and graduate students. Researchers in other fields with some interest in cosmochemistry will also find this book extremely useful.

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1 McSween HY Jr, Huss GR (2010) Cosmochemistry. Cambridge University Press Cambridge, ISBN 978-0-52187-862-3; £45.00 (US$78.00)

THEORETICAL AND COMPUTATIONAL METHODS IN MINERAL PHYSICS: GEOPHYSICAL APPLICATIONS[2]

In the foreword to Reviews in Mineralogy and Geochemistry volume 71, entitled *Theoretical and Computational Methods in Mineral Physics: Geophysical Applications*, the editors, Renata Wentzcovitch and Lars Stixrude, note that the influence of computational mineral physics to the Earth sciences has been "transformative and was unimaginable at the onset." Just how much the use of atomistic model calculations in the mineral sciences has changed in the last 25 years becomes clear by comparing volume 71 with volume 14 of the series, published in 1985 (*Microscopic to Macroscopic: Atomic Environments to Mineral Thermodynamics*; S.W. Kieffer and A. Navrotsky, editors). While atomistic model calculations have long been employed to study structure–property relations of a few minerals (e.g. by Born and Zeman in 1963 for garnets), in the mid-1980s atomistic modeling of minerals emerged as a tool to understand and predict structures, stabilities, and elastic, vibrational, and thermodynamic properties of silicates and related compounds. Volume 14 includes a paper by Burnham, entitled "Mineral Structure Energetics and Modeling Using the Ionic Model," which describes the state of the art at that time.

Volume 71 shows that models based on empirical potential (force field) are still employed to give fundamental insight that cannot be obtained by models based on quantum mechanics due either to the number of atoms required in the simulation or to the requirement for very fast calculations. For example, in molecular dynamics simulations, millions of time steps maybe required. Twenty years ago a simple geometric optimization of an ionic model of garnet on a microVax using one of the few established codes at that time took a few days. Nowadays, the same calculation takes a few seconds on a PC. These advancements are due not only to improvements in the hardware but also to the development of very efficient codes, such as the very widely used "General Utility Lattice Program" (GULP), written by J. Gale. The capabilities of this program are introduced in a chapter by J. Gale and K. Wright. In other chapters (Carrez and Cordier on dislocation modeling, Vinograd and Winkler on modeling of the thermodynamics of solid solutions), applications of atomistic modeling studies performed with the GULP code are presented; in these applications, rather complex structural models are required, thus preventing the brute-force approach used with quantum mechanical models. The usefulness of force field calculations is also discussed by Ghiorso and Spera, who employ models with several thousand atoms, running for long times, to study transport properties.

So, while more mature, user-friendly, and efficient codes, in conjunction with faster computers, have transformed the field of empirical potential–based modeling, this development could have been anticipated 25 years ago. The most fundamental change, which was not foreseeable 25 years ago, was the impact that density functional theory (DFT)–based calculations have nowadays. DFT-based calculations of structures and their properties are currently the most widely used quantum mechanical models for solids, and they have provided new insight into all fields concerned with the understanding of structure–property relations of condensed matter. Consequently, the book provides overviews to the theoretical groundwork of DFT (by Perdew and Ruszsinsky) and to density functional perturbation theory (by Baroni et al.). The latter is an extension of "standard" DFT that allows an efficient calculation of the lattice dynamics, and hence of thermodynamic properties, in the quasi-harmonic approximation. These two chapters provide a good entry point for researchers interested in the foundation of modern atomistic simulation approaches. A chapter entitled "Minnesota Density Functionals" (by Zhao and Truhlar) is addressed more to the advanced specialist as, to the best of my knowledge, their functionals have not yet been implemented in DFT codes commonly used in mineral physics studies.

After introducing the theoretical basis, emphasis is placed on studies showing state-of-the-art developments of approaches needed to compute thermodynamic and thermoelastic properties (chapters by Wentzcovitch at al.; Alfe; and Stixrude and Lithgow-Bertelloni), diffusion (Amman et al.), thermal conductivity (Stackhouse and Stixrude), structure prediction (Oganov et al.), and phase transition in ice and at multi-megabar pressures (chapters by Umemoto and Umemoto et al.). It is worthwhile noting that the studies of dislocations and solid solutions mentioned above also employed density functional theory–based calculations at some stages, e.g. for validating empirical potentials. The ability to compute structures and properties at elevated temperatures, and not only in the athermal limit, is of fundamental importance for the applicability of first-principles calculations to the Earth sciences, and the book conveys in an outstanding manner the achievements of the last years.

In addition to the studies mentioned above, which are mostly concerned with crystalline phases, DFT studies also allow the simulation of melts (chapter by Karki). A comparison with the Ghiorso and Spera contribution highlights the difference between force field–based models and parameter-free DFT simulations with respect to accessible ensemble sizes and simulation times. The comparatively small ensembles that can be studied by quantum mechanical methods require extensive tests to exclude size effects, i.e., the dependence of the results on the number of atoms used in the model. On the other hand, the predictive power of force fields is limited to the pressure range for which they were derived, and the applicability of such models in simulations of the behavior of minerals at extreme conditions requires extensive validation studies, so that parameter-free models become a more attractive choice. It will be interesting to see how far and how fast the gap between force field models for molecular dynamics simulations and *ab initio* calculations will be closed by the evolution of new hardware concepts, such as the use of graphical processing units, in conjunction with new parallelization techniques.

While the above-mentioned chapters convincingly show that with "standard" DFT numerous problems can be addressed, this approach has several shortcomings, many of which are related to our ignorance of the exact form of the exchange-correlation functional. This lack of knowledge forces us to use approximations such as the generalized gradient approximation. It is therefore of great interest to develop alternative methods that do not rely on approximations. One such approach is based on quantum Monte Carlo (QMC) techniques, introduced in the contributions by Ceperley and Mitas and Kolorenc. There is, of course, the caveat "Given sufficient computer resources…", which is a subtle hint to the adventurous reader who is considering trying this approach, that these calculations can be computationally very expensive, and the codes are certainly not as easy to use as some of the mature DFT codes available in the public domain.

Alternatively, some shortcomings of standard DFT approaches can be overcome by an extension of standard DFT, and one such extension, the so-called LDA+U approach, is reviewed by Cococcini. In the Earth sciences, this approach, which better describes the interaction of localized electrons, is required for accurate studies of several important iron-containing phases, such as wüstite and fayalite, and specifically for studies of spin transitions of lower-mantle minerals (chapter by Hsu et al.).

As is obvious from this long list of topics, volume 71 provides a comprehensive overview of recent developments in atomistic modeling approaches in mineral physics. The editors have very carefully selected complementary contributions from leaders in the field, which cover the general topic from a variety of viewpoints. There is very little redundancy. The contributions are balanced, although other approaches, such as the calculation of phonons from finite displacements instead of perturbation theory, could have been included. It probably would have been helpful for some readers to have a list of Internet resources, as many codes are in the public domain, and excellent tutorials are available on the web. But these are minor shortcomings, as the extended bibliographies contain all the necessary information.

In conclusion, volume 71 of Reviews in Mineralogy & Geochemistry offers a representative snapshot of the current state-of-the-art computational methods in mineral physics. Comparing volume 14 to volume 71 leads me to wonder about the unforeseen developments that volume 137, to be published around 2035, will contain.

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2 Wentzcovitch R, Stixrude L (eds) 2010 Theoretical and Computational Methods in Mineral Physics: Geophysical Applications. Reviews in Mineralogy and Geochemistry 71, Mineralogical Society of America, Chantilly, VA, 484 pages, ISBN 978-0-939950-85-0, US$40 (25% off for MSA and GS members)