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The Future of High-Pressure Mineral Physics

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Research in mineral physics is essential in interpreting observational data from many other disciplines in the Earth sciences, including geodynamics, seismology, geochemistry, petrology, geomagnetism, and planetary science, as well as materials science and climate studies, as illustrated in Figure 1. The field of high-pressure mineral physics is highly interdisciplinary and fundamentally multidisciplinary. Mineral physicists do not always study minerals or use only physics; they study the science of materials that compose the Earth and other planets, and employ concepts and techniques from chemistry, physics, materials science, and biology.

A dramatic example of this interdisciplinarity in action occurred during the past year. The experimental discovery and theoretical confirmation in 2004 of a new phase of magnesium metasilicate ($MgSiO_3$) stable only at pressures above 100 Gigapascals (and termed the postperovskite phase) has had an immediate and profound impact on multidisciplinary studies of the deep mantle of the Earth (see article by Lay et al. in the 4 January 2005 issue of *Eos*).

As those authors state, "…the characteristics of this phase transition indicate that it may hold the key to understanding enigmatic seismological structures in the D" region of the lowermost mantle, with important implications for heat transport, thermal instabilities, and chemical properties of the lower mantle." Figure 2 shows the crystal structure of the newly discovered postperovskite phase of $MgSiO_3$, and also includes a representational sketch of complexities in deep-mantle structure beneath South Africa.

Among the current research topics receiving considerable attention in the field of mineral physics are the following: (1) the incorporation of water, carbon, and other volatiles into high-pressure phases, and the influence of these volatiles on physical properties (e.g., transport and thermoelastic) and deep Earth processes (e.g., kinetics and mechanisms of phase transitions and melting relations); (2) the valence and spin configuration of iron in the mineral phases in the Earth's mantle; (3) simultaneous studies of the elasticity and equation of state (relationship between pressure-volume-temperature) of solids at high pressures and temperatures using acoustic techniques in conjunction with X-ray synchrotron radiation; (4) rheological investigations at conditions of the transition zone of the mantle and below; and (5) the role of clathrates, or solid gas hydrates, in influencing processes in the interiors of planets. Studies on each of these topics have broad interdisciplinary importance across the fields shown in Figure 1.

Challenges in the 21st Century

The field of high-pressure Earth and planetary sciences has changed dramatically over the past decade. Increasingly sophisticated tools are being used to investigate the properties of matter under the extreme pressure and temperature conditions of planetary interiors. Similar progress has been achieved in the computational power for calculations of mineral properties. As a result, it is now possible to do experiments and perform simulations that were not dreamed of 10 years ago.

Many of these advances and prospects for the future have been described in a recent report, "Current and future research directions in high-pressure mineral physics." The report was edited by Jay Bass with the support of the Consortium for Materials Properties Research in Earth Sciences (COMPRES) and the U.S. National Science Foundation (NSF).

The report is intended to be a statement by the high-pressure Earth science community on the status of this field and some of its most exciting and challenging research directions for the near future. A poster illustrating the

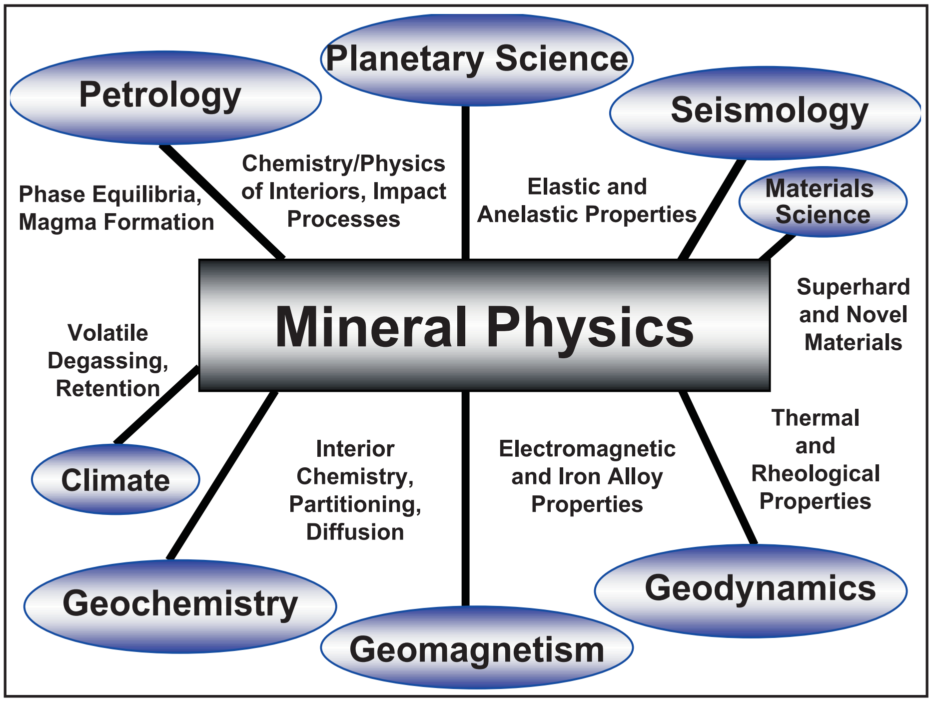

Fig. 1. Links of mineral physics with other Earth science fields.

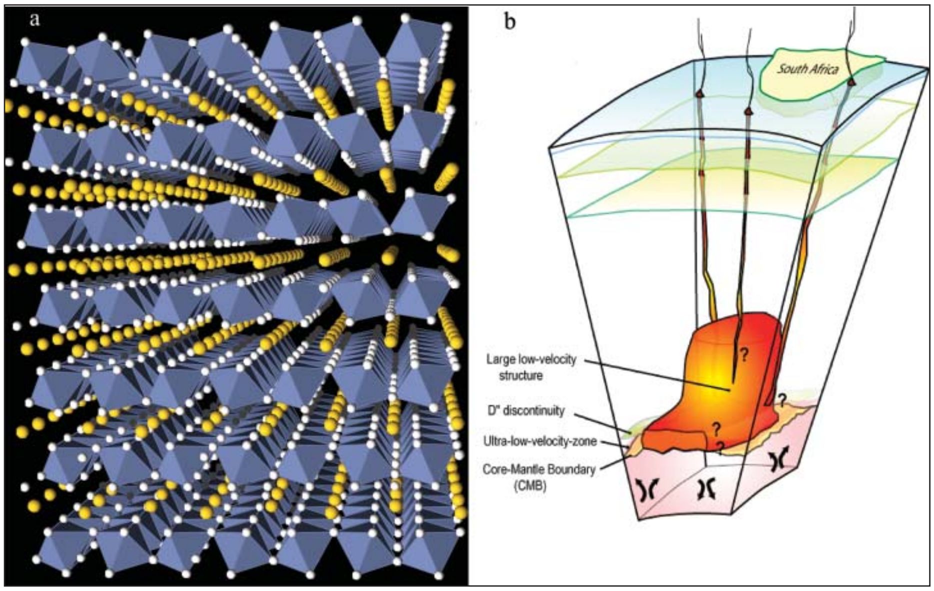

Fig. 2. Hybrid figure including (a) the crystal structure of postperovskite $MgSiO_3$ [from Murakami et al., *2004] and (b) the deep mantle structure under South Africa [from* Garnero, *2004].*

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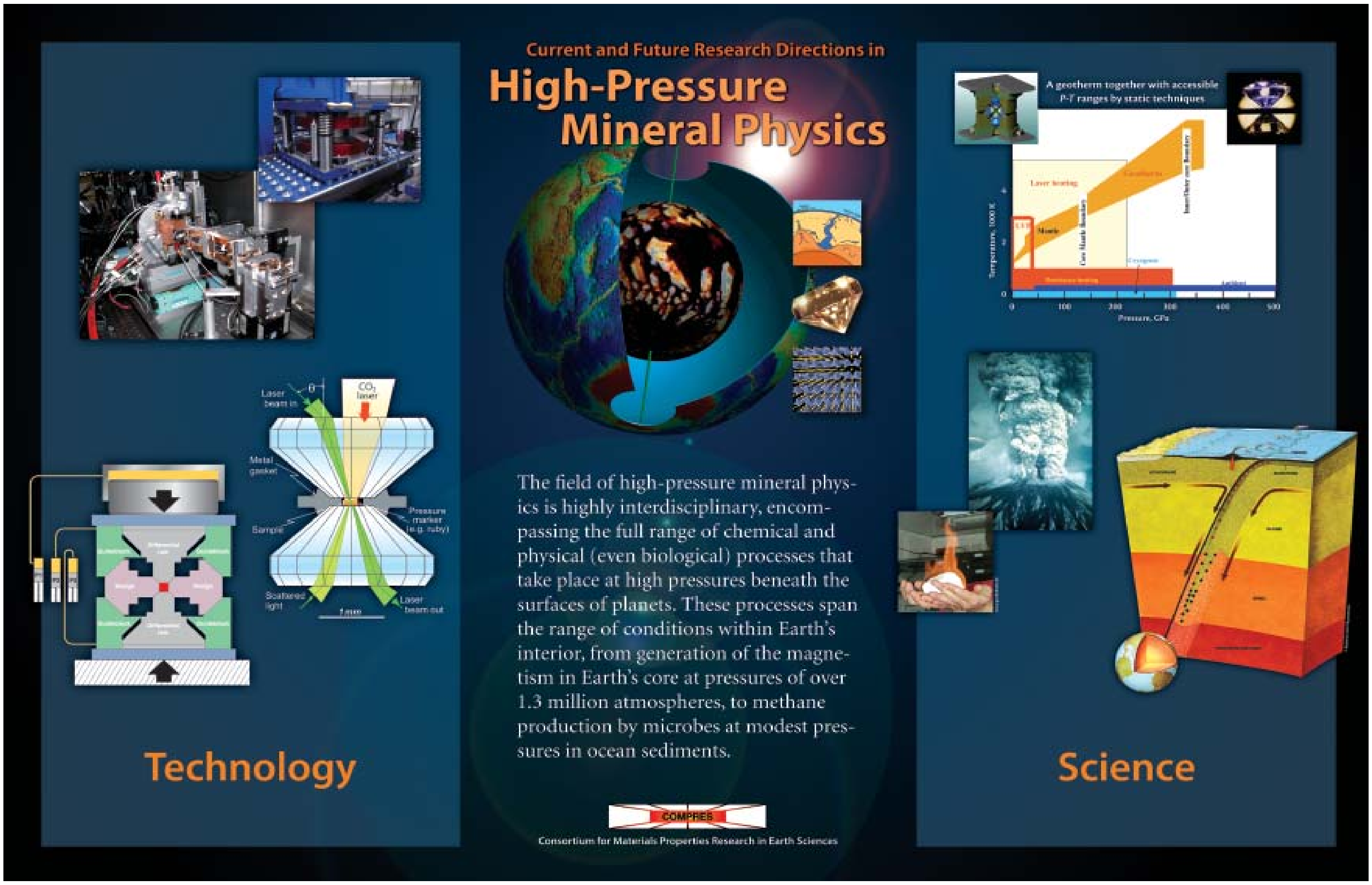
Current and Future Research Directions in
High-Pressure
Mineral Physics

The field of high-pressure mineral physics is highly interdisciplinary, encompassing the full range of chemical and physical (even biological) processes that take place at high pressures beneath the surfaces of planets. These processes span the range of conditions within Earth's interior, from generation of the magnetism in Earth's core at pressures of over 1.3 million atmospheres, to methane production by microbes at modest pressures in ocean sediments.

Technology

Science

COMPRES
Consortium for Materials Properties Research in Earth Sciences

Fig. 3. Poster illustrating Current and Future Research Directions in High-Pressure Mineral Physics (COMPRES).

central themes of the Bass report is shown in Figure 3. Copies of this report and the poster are available at http://www.compres.us from COMPRES administrative coordinator Ann Lattimore (ESS Building, Stony Brook, N.Y. 11794-2100; E-mail: alattimore@notes.cc.sunysb.edu).

At the onset of the 21st century, mineral physicists find themselves with many challenging research problems and exciting opportunities for research at high pressures and temperatures, made possible in large measure by the availability of synchrotron and neutron facilities at the national laboratories of the U.S. Department of Energy (DOE).

In parallel with these advances in large, centralized facilities, new types of high-pressure devices, of both the diamond-anvil and multianvil types, have been developed to take advantage of them. To exploit such technologies requires a change in the culture of high-pressure experimental research. Until recently, the cottage industry model served as the primary mode of operation: A scientist worked with a student and/or a postdoc, together in a laboratory at their home institution.

The new, centralized national facilities demand a different strategy that includes advanced preparation of samples and experiments, weeks in the "field" (at the national facility), sleepless nights, and compact discs full of data. Following the experiments, the fatigued team returns home for weeks of data analysis.

This new mode requires re-education to enable all scientists, from student to senior faculty, to effectively participate in this new culture. A community-based approach to organizing these scientific efforts was clearly called for.

Role of COMPRES

COMPRES was formed in part as a response to these new scientific and technological developments and new styles of conducting high-pressure science. Starting with a Town Meeting at the 2000 AGU Fall Meeting, in San Francisco, organized by the AGU Mineral and Rock Physics Committee, the planning process began in earnest with a workshop at the Scripps Institution of Oceanography, in La Jolla, California, in February 2001. The process culminated in a successful proposal to the NSF Division of Earth Sciences in August 2001. In May 2002, a cooperative agreement was promulgated that projected funding for COMPRES for a five-year period to April 2007.

COMPRES currently has 44 members that are educational or governmental institutions in the United States with research and educational programs in high-pressure research in the science of Earth materials. There are also 16 foreign affiliate institutions.

COMPRES supports the operations of high-pressure beam lines at synchrotrons to provide access and support to students and staff scientists in the Earth science community. These operations include (1) diamond-anvil facilities at the National Synchrotron Light Source (NSLS) of the Brookhaven National Laboratory, New York; (2) multi-anvil facilities at the NSLS; and (3) diamond-anvil facilities at the Advanced Light Source of the Lawrence Berkeley National Laboratory, California.

COMPRES also supports a neutron studies initiative to cultivate scientific interest in exploiting the new opportunities to come in 2008 at the Spallation Neutron Source of the Oak Ridge National Laboratory, Tennessee, and coordinates its activities with those of theGeoSoil-EnviroCARS, a synchrotron-based facility at the Advanced Photon Source of the Argonne National Laboratory, Illinois.

In addition to the operation of community facilities, COMPRES supports infrastructure projects to promote the development of new technologies for high-pressure research, both in laboratories, in home institutions, and at DOE national laboratories. COMPRES also advocates for science and educational programs to the various U.S. funding agencies, including NSF, DOE, the Department of Defense, and NASA.

The community-wide organization of mineral and rock physics introduced by COMPRES is analogous to the centralization of efforts in other geophysical sciences, such as the coordination of seismic data distribution and instrument deployment orchestrated by the Incorporated Research Institutions of Seismology.

The two major COMPRES programs for Community Facilities Operations and Infrastructure Development Projects are overseen by two standing committees, which are elected by representatives of U.S. member institutions.

Under separate funding from the NSF Division of Earth Sciences, scientists in the COMPRES community are pursuing three grand challenge collaborative research programs: growth of large synthetic diamonds by chemical vapor deposition, rheology of Earth materials, and elasticity of Earth materials—all at high pressures and temperatures.

While these grand challenge programs are formally independent of the COMPRES core grant, they are intellectually related, as they provide prime examples of the scientific problems that can be addressed using the community facilities operated by, and the technological developments funded by, COMPRES.

Communication within the mineral physics community includes monthly letters from the president, quarterly newsletters, an active Web site (http://www.compres.us), and an annual meeting. The 2005 annual meeting of COMPRES was held in New Paltz, New York, on 16–19 June and attracted 108 participants; it included focus sessions on the mantle, the core, and geochemical evolution, with keynote talks followed by group discussion. The meeting also featured reports from the Community Facilities operations and Infrastructure Development projects and poster presentations highlighting some exciting recent scientific achievements.

Acknowledgments

I am indebted to Jay Bass and Donald Weidner for their permission to borrow some material from the Bass report and the original COMPRES proposal to the NSF. I am also grateful to Harry Green, Shun Karato, Charles Prewitt, and Quentin Williams for their perceptive comments and useful suggestions for modifications to earlier versions of this report, and to Ann Lattimore for creating Figure 1. This report has been prepared by, and is being submitted on behalf of, the COMPRES community. The author is the president of COMPRES and has no direct relationship with any of the DOE national laboratories referred to in this report.

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Arctic Ocean Study: Synthesis of Model Results and Observations

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Model development and simulations represent a comprehensive synthesis of observations with advances in numerous disciplines (physics; mathematics; and atmospheric, oceanic, cryospheric, and related sciences), enabling hypothesis testing via numerical experiments. For the Arctic Ocean, modeling has become one of the major instruments for understanding past conditions and explaining recently observed changes.

In this context, the international Arctic Ocean Model Intercomparison Project (AOMIP, http://fish.cims.nyu.edu/project_aomip/overview.html) has investigated various aspects of ocean and sea ice changes for the time period 1948 to present. Among the major AOMIP themes are investigations of the origin and variability of Atlantic water (AW) circulation, mechanisms of accumulation and release of fresh water (FW), causes of sea level rise, and the role of tides in shaping climate.

This article presents several hypotheses based on the synthesis of model results with observations, and it delineates major directions for modeling studies during the International Polar Year (IPY) 2007–2008.

Atlantic Water Circulation

The puzzle of AW circulation at 200–800 m depth has been studied by generations of Arctic scientists. AW penetrates into the Arctic via Fram Strait and St. Anna Trough (Barents Sea). Under extensive surface cooling, it sinks to intermediate depths and forms the relatively warm Atlantic Layer ($\Theta > 0°C$, where Θ represents potential water temperature). This layer is covered by low-density surface waters and is thus prevented from undergoing heat and momentum exchange with the atmosphere.

The most widely accepted theory postulates that AW circulates counterclockwise in the Arctic basins (Figure 1). Among AOMIP models, the simulated AW circulation differs in intensity and sense of rotation: Some models show anticyclonic and some support cyclonic circulation patterns. AOMIP has examined the underlying causes for such inconsistency, identified factors influencing AW behavior, and formulated important implications from these studies.

In an idealized model, J. Yang (Woods Hole Oceanographic Institution; see the AOMIP Web site for all article references) examined how flux of potential vorticity (PV) at the Arctic Ocean boundaries affects the AW circulation direction. Because AW is not directly forced by wind stress, the PV integral over the Arctic basins yields a balance between the net lateral PV inflow through straits and PV dissipation along the boundary. When a layer between two surfaces of constant density receives net positive (negative) PV through inflow or outflow, the circulation becomes cyclonic (anticyclonic) so that friction can generate a flux of negative (positive) PV to satisfy the integral balance.

A significant implication is that the hydrographic structure and transport of AW entering or leaving the Arctic are important for setting the pattern and direction of AW circulation, and that long-term, high-resolution, year-round monitoring of boundary throughflow is needed for understanding and predicting AW characteristics.

A different idea by G. Holloway (Institute of Ocean Sciences, Sidney, Canada) is that eddy generation of entropy drives cyclonic boundary currents around the Arctic basins, implying that the cyclonic circulation should be relatively persistent even under changing boundary conditions.

Furthermore, AOMIP numerical experiments reveal that excessive mixing leads to a breakdown or reversal of AW circulation, because a strong surface anticyclonic Beaufort Gyre can weaken the cyclonic AW flow at mid-depth. It was found that the AW circulation has a pulsating character expressed in the propagation of warm and cold events, varying on seasonal to decadal timescales. Collaborating with the Arctic/Subarctic Ocean Fluxes (ASOF) and Nansen and Amundsen Basins Observing System programs, AOMIP models are being used to elucidate the predictive potential for AW flow. Theoretical and modeling studies are also used to identify specific conditions sufficient to reverse AW circulation.

Mechanism of Fresh Water Accumulation and Release

The meridional overturning circulation in the Atlantic Ocean is significantly influenced by FW fluxes from the Arctic Ocean. The international programs Community-Wide Hydrological Analysis and Monitoring Program (CHAMP) and ASOF were organized with the major goal of investigating these fluxes and the FW balance of the Arctic Ocean. As a participant in CHAMP, A. Proshutinsky, lead author of this article and AOMIP principle investigator, proposed and demonstrated that the Arctic Ocean can accumulate a significant amount of FW during anticyclonic circulation regimes and release this water to the North Atlantic during cyclonic regimes.

The Beaufort Gyre of the Canada Basin contains approximately 45,000 km^3 of FW, a volume 10–15 times larger than the total annual river runoff to the Arctic Ocean, and larger than the amount of FW stored in the sea ice. A release of only 5% of this FW is enough to cause salinity anomalies in the North Atlantic, as observed in the 1970s. Because the Beaufort Gyre is the major reservoir of FW

By A. Proshutinsky, J. Yang, R. Krishfield, R. Gerdes, M. Karcher, F. Kauker, C. Koeberle, S. Hakkinen, W. Hibler, D. Holland, M. Maqueda, G. Holloway, E. Hunke, W. Maslowski, M. Steele, and J. Zhang