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Mineral Physics

Robert Cooper Liebermann

Abstract

Mineral physics emerged as an independent discipline of Earth sciences in the middle of the 20th century, drawing together geophysics and mineralogy. Using the principles of condensed matter physics and solid-state chemistry, it focuses on exploring how physical properties of minerals depend on atomic structure. With the advent of new experimental tools (e.g., automated X-ray diffractometers, electron microscopes, various spectrometric techniques, digital computers and synchrotron X-radiation sources) in the past 70 years, geophysicists and mineralogists began to talk with one another.

Keywords: mineral physics, geophysics, mineralogy, high pressure, high temperature, applications to earth

1. Introduction

In the 1960s, Orson Anderson established a new laboratory at Columbia University's Lamont Geological Observatory and chose to name it "Mineral Physics." Experiments in his laboratory measured mineral properties over the wide range of pressures, temperatures and chemical compositions seen in the interior of Earth and other terrestrial planets. These studies included properties of minerals, but all materials related to natural minerals (e.g., structural analogs, but also glasses, melts and fluids). According to Robert Hazen [1], "mineral physics is the study of mineralogical problems through the application of condensed matter physics". In reality, mineral physicists use not only physics but also solid-state chemistry. Knowledge of these properties is essential to interpretations of seismic data accurately and performing realistic geodynamic simulations. Today, mineral physics is widely considered one of the three pillars of geophysics, along with geodynamics and seismology.

Today, scientists approach these problems through a combination of experimental and computational methods. Precise information at lower pressures and temperatures is provided by experiments, and detailed information at conditions difficult to re-created in the laboratory is provided by computational work. Bulk material properties are vital to understanding the behavior of planets, but atomistic inspection of these complex materials provides a connection to planetary-scale phenomena. Theoretical mineral physicists are in a unique position to illuminate this connection [2] (see also paragraph by Taku Tsuchiya below).

In the past half century since the first scientific conference focused on mineral physics was held in 1977, mineral physics has matured into an independent scientific discipline firmly in the mainstream of geosciences. Now mineral physicists are faced with many challenging problems and many exciting opportunities for research; in large

measure, this is now possible due to access to synchrotron X-radiation facilities throughout the world. This evolution is highlighted in this chapter (see also our earlier paper [3]).

2. History prior to the 1950s

Long before seismology became a recognized discipline early in the 20th century, many scientists and philosophers had speculated on the nature of the interior of Earth. One of the earliest of these was Athanasius Kircher (1602–1680) whose view of Earth (**Figure 1**) was published in 1665 and entitled: *Mundus Subterraneus* [4].

Over the subsequent three centuries as more detailed information became available from improved scientific methods, especially in seismology, our view of the interior of Earth has evolved, but major features have remained unchanged (**Figure 2**).

Harvard University faculty dominated investigations of the problems related to mineral physics in the first half of the 20th century. The first was Percy Bridgman whose investigations of the properties of matter under high pressure earned him the Nobel Prize in Physics in 1946. Among the graduate students of Bridgman was Francis Birch, who focused on high-pressure studies relevant to geophysical problems. In his classical paper in 1952 [5], he demonstrated that the mantle is predominately composed of silicate minerals and that the upper mantle and lower mantle regions, each essentially homogeneous but of somewhat differing compositions, are separated by a thin transition zone associated with silicate phase transitions (see green band at 670 km in **Figure 3**). Birch also concluded that the inner and outer core are alloys of crystalline and molten iron, respectively, which contrasted with the prevailing views at the time. Although a few refinements have become necessary in light of subsequent research, the essential details of this model are still valid. For this paper and other contributions, Birch is widely acknowledged as the “father of mineral physics” (though he never used that term).

Figure 1.
View of earth in 1665 by Athanasius Kircher (1602–1680).

Figure 2.
Views of the interior of the earth from 1665 to 1990. Courtesy of Ed Garnero.

Figure 3.
Internal structure and composition of the Earth's interior.

3. Post 1950s developments

Over the last four decades of the 20th century, many laboratories in the United States, Japan, Australia and France began to conduct experiments on the physical properties of minerals at high pressures and temperatures. These laboratories focused their research on understanding the role of fundamental properties of minerals and thus provided links to other disciplines of the geosciences such as seismology, tectonophysics, volcanology, geochemistry and petrology. These links are graphically illustrated by **Figure 4**.

Figure 4. Williams-Lattimore diagram reflecting the relationship of mineral physics to other disciplines of geosciences (copyright R. C. Liebermann).

4. Inventions of DACs and MAA

In the past 50+ years, two major static high-pressure techniques have been developed in mineral physics laboratories by earth scientists desiring to replicate in the laboratory the P-T conditions of Earth's deep interior: the diamond-anvil cell (DAC) and the multi-anvil apparatus (MAA). These two static techniques are both useful and very complementary, although have occasionally been viewed as competitive. Higher pressures and large sample volumes can be achieved either through the use of larger tonnage hydraulic rams in MAAs or by increasing the culet size of DACs, and thus experimental conditions of the two techniques will eventually merge.

(a)

(b)

Figure 5.
a. Geotherm with P - T ranges compared with the P - T regions achievable with diamond anvil cells (and various types of heating) and with LVP (large-volume presses, aka multi-anvil apparatus). *b.* Temperature and pressures achievable in difference types of large-volume apparatus.

The diamond-anvil cell (DAC) was invented at the National Bureau of Standards [NBS] under the direction of Alvin Van Valkenburg and his colleagues in 1958. For the subsequent developments of the DAC, see the excellent review by William Bassett [6]. In the same time period, Tracy Hall invented the first multi-anvil apparatus, a tetrahedral-anvil machine; such MAA have evolved progressively [7] and can now achieve pressures close to 100 GPa at high temperatures. With the advent of synchrotron radiation facilities in the early 1980s, many of these DAC and MAA devices have been utilized in conjunction with *in situ* X-ray diffraction.

In **Figure 5a** and **b**, we illustrate the pressure and temperature ranges achievable with the diamond anvil cells and multi-anvil apparatus and compare those with the P–T ranges of the geotherm of the Earth.

In **Figure 6**, the regions of the Earth's interior (Crust, Upper mantle, Lower mantle, Outer core and Inner core) accessible to different types of high-pressure apparatus: Belt, Split-Sphere, DIA and DAC are illustrated.

With the aid of high-pressure devices such as diamond anvil cells and multi-anvil apparatus, scientists have been able to explore the crystallographic transformations which the principal minerals of the upper mantle undergo as they are buried deeper in the Earth's interior. Thus, olivine, garnet, clinopyroxene and orthopyroxene of the upper mantle evolve to mixtures of (Mg, Fe)O-ferropericlase and Ca- and (Mg, Fe, Al)-SiO₃-perovskites [the latter recently named bridgmanite] in the lower mantle. In the vicinity of the outer core, the bridgmanite transforms to a post-perovskite phase which has not yet been found in nature (see **Figure 7a**, courtesy of Stas Sinogeikin and **Figure 7b**, courtesy of Nick Schmerr and Ed Garnero).

In addition to experiments using static multi-anvil apparatus or diamond anvil cells, many scientists have utilized dynamic shock wave techniques to measure the physical properties of minerals at high pressures and temperatures. In **Figure 8**, the shock wave gun at Caltech is shown; it was originally built by Thomas Ahrens and is now under the supervision of Paul Asimow.

High Pressure Instrumentation

Figure 6. Regions of the Earth's interior accessible to different types of high-pressure apparatus: Belt, Split-sphere, DIA and DAC.

Figure 7.
a. Evolution of minerals in the earth from the upper mantle to the core. Courtesy of Stas Sinogeikin. b. Upper mantle seismic discontinuities: Mineral phase boundaries. Courtesy of Nick Schmerr and Ed Garnero.

In a paper now in press entitled “New analysis of shock-compression data for selected silicates”, Thomas Duffy has illustrated one of the important uses of shock wave experiments:

“The study of minerals under shock compression provides fundamental constraints on their response to conditions of extreme pressure, temperature, and strain rate and has applications to understanding meteorite impacts and the deep Earth. The recent development of facilities for real-time *in situ* X-ray diffraction studies under gun- or laser-based dynamic compression provides new capability for understanding

Figure 8.

Static (multi-anvil press and diamond anvil cell) high-pressure devices illustrated with the dynamic shock-wave gun at Caltech.

the atomic-level structure of shocked solids. Here traditional shock pressure-density data for selected silicate minerals (garnets, tourmaline, nepheline, topaz, and spodumene) are examined through comparison of their Hugoniot with recent static compression and theoretical studies. The results provide insights into the stability of silicate structures and the possible nature of high-pressure phases under shock loading. This type of examination highlights the potential for *in situ* atomic-level measurements to address questions about phase transitions, transition kinetics, and structures formed under shock-compression for silicate minerals.”

Experiments are not the only solution to finding progress. In the figure above is a quote by Artem Oganov:

“High-pressure experiments are extremely difficult”.

Thus, he resorts to the computer for theoretical calculations.

“Recent progress in theoretical mineral physics based on the *ab initio* quantum mechanical computation method has been dramatic in conjunction with the rapid advancement of computer technologies. This technique solves electronic structures and chemical bonding natures of materials highly accurately and became practical after the beginning of this century. It is now possible to predict thermodynamic stability, elasticity, and transport properties of complex minerals quantitatively with uncertainties that are comparable or even smaller than those attached in experimental data under high pressure and high temperature. These calculations under *in situ* high-pressure (P) and high-temperature (T) condition allow us to construct *a priori* mineralogical models of the deep Earth and have opened a new generation in solid geophysics and geochemistry”. (Taku Tsuchiya, personal communication, 2021).

5. Experimental physical acoustics and elasticity of minerals

Experimental physical acoustics has been used to study the elastic properties of minerals. These high-precision techniques provide measurements of the velocity of sound in single crystals or polycrystalline aggregates (i.e., rocks) as functions of pressure and temperature.

There are several goals of such research in geophysics:

- a. To study the relationship of the elastic properties to crystallographic structure and composition.
- b. To provide the input parameters for theoretical equations of state of solids to enable these ultrasonic data to be extrapolated to higher pressures and temperatures, and
- c. To deduce the composition and mineralogy of the Earth's interior from a comparison of the laboratory data with the velocity-depth profiles in the Earth derived from seismology.

Our recent paper [8] summarizes the current state-of-the-art in studies of the Earth's interior using measurements of sound velocities in minerals by ultrasonic interferometry. In that paper, we reviewed the progress of the technology of ultrasonic

Figure 9.
Comparison of seismic models (PREM-dashed lines and AK135-solid lines) with possible mineral phase transitions in the minerals of the upper mantle (see also **Figures 3 and 7a, b**).

Figure 10.
The progress in the pressures and temperatures achievable in these investigations using laboratory acoustics from 1994 to 2014 is reflected in these three figures.

interferometry from the early 1950s to the present day. During this period of more than 60 years, sound wave velocity measurements have been increased from pressures less than 1 GPa and temperatures less than 800 K to conditions above 25 GPa and temperatures of 1800 K. This is complimentary to other direct methods to measure

sound velocities (such as Brillouin spectroscopy and impulsive stimulated scattering) as well as indirect methods (e.g., resonance ultra-sound spectroscopy, static or shock compression, inelastic X-ray scattering). Newly-developed pressure calibration methods by Wang *et al.* [9] and data analysis procedures using a finite strain approach are described and applied to data for the major mantle minerals. These state-of-the-art ultrasonic experiments performed in conjunction with synchrotron X-radiation provide simultaneous measurements of the elastic bulk and shear moduli and their pressure and temperature derivatives with direct determination of pressure.

These sound velocity data are important in enabling scientists to interpret seismic data for the Earth's interior. Two of the most popular global seismic models are PREM and AK135 [10, 11] are plotted in **Figure 9**; these models include some distinct features including a low velocity zone around 80 km–150 km, jumps at 410- and 670-km depths, and high velocity gradients in the transition zone. In addition, regional seismic studies also revealed discontinuities at 520 km as well as at depths of 250 km–340 km (X discontinuity). Also plotted are phase transitions as possible causes of these velocity anomalies in a pyrolytic mantle compositional model (See **Figure 9** and **Figures 3** and **7a** and **b** above).

The progress in the pressures and temperatures achievable in these investigations using laboratory acoustics from 1994 to 2014 is reflected in the following figures (**Figure 10**); copyright R. C. Liebermann.

6. Current status of mineral physics research

In early 2019, I wrote a paper entitled “The Orson Anderson Era of Mineral Physics at Lamont in the 1960s”, and began to explore options for its publication. When the Assistant Editor for Minerals, Ms. Jingjing Yang, agreed to consider my paper, she also inquired as to whether I would like to be the Guest Editor for a Special Issue in honor of Orson Anderson. After asking prospective authors about the viability of such a Special Issue, I accepted her invitation, with the hope and expectation that it would be a wonderful present for his 95th birthday. This Special Issue is the result [12]. It contains original scientific papers, as well as historical reviews of the field of mineral physics (and also rock physics).

The papers in this Special Issue are grouped into four categories: Reviews, Experimental Science, Theoretical Science and Technological Developments. These papers include those from; first authors covering five generations of mineral physicists, including contemporaries of Orson, the next generation of leaders in mineral physics throughout the world, current leaders in the field, senior graduate students, and an undergraduate student (i.e., Tyler Perez). Note that Tyler, a student of Jennifer Jackson at Caltech, is an academic great-great grandson of Orson Anderson (Anderson > Liebermann > Bass > J. Jackson > Perez).

Examples of papers in all four categories of the Special Issue [12]:

7. Review

William A. Bassett.

The Takahashi–Bassett Era of Mineral Physics at Rochester in the 1960s. Reprinted from: Minerals 2020, 10, 344, doi:10.3390/min10040344

8. Experimental science

Agnés Dewaele.

Equations of State of Simple Solids (Including Pb, NaCl and LiF) Compressed in Helium or Neon in the Mbar Range, Reprinted from: Minerals 2019, 9, 684, doi:10.3390/min9110684

Tyler Perez, Gregory J. Finkelstein, Olivia Pardo, Natalia V. Solomatova and Jennifer M. Jackson.

A Synchrotron Mössbauer Spectroscopy Study of a Hydrated Iron-Sulfate at High Pressures Reprinted from: Minerals 2020, 10, 146, doi:10.3390/min10020146

Francesca Miozzi, Jan Matas, Nicolas Guignot, James Badro, Julien Siebert and Guillaume Fiquet.

A New Reference for the Thermal Equation of State of Iron, Reprinted from: Minerals 2020, 10, 100, doi:10.3390/min10020100

9. Theoretical science

J. Michael Brown and Baptiste Journaux.

Local-Basis-Function Equation of State for Ice VII–X to 450 GPa at 300 K, Reprinted from: Minerals 2020, 10, 92, doi:10.3390/min10020092

Jun Tsuchiya, Risa Nishida and Taku Tsuchiya.

First Principles Calculation of the Stability of Iron Bearing Carbonates at High Pressure Conditions, Reprinted from: Minerals 2020, 10, 54, doi:10.3390/min10010054

10. Technological developments

Tony Yu, Clemens Prescher, Young Jay Ryu, Feng Shi, Eran Greenberg, Vitali Prakapenka, Peter Eng, Joanne Stubbs, Yoshio Kono, Guoyin Shen, Heather Watson, Mark L. Rivers, Stephen R. Sutton and Yanbin Wang.

A Paris-Edinburgh Cell for High-Pressure and High-Temperature Structure Studies on Silicate Liquids Using Monochromatic Synchrotron Radiation, Reprinted from: Minerals 2019, 9, 715, doi:10.3390/min911071

Acknowledgements

I am grateful to William Bassett, Thomas Duffy and Taku Tsuchiya for their contributions to the sections on diamond anvil cells, shock waves and theoretical mineral physics, respectively. I appreciate the courtesy of many colleagues in providing figures to illustrate this paper: Ed Garner, Quentin Williams, Guoyin Shen, Shun Karato, Nick Schmerr and Stas Sinogeikin; all colleagues have granted explicit permission to use their figures in this chapter, none of which have been published. Portions of this chapter have been adapted and modified from the author's previous publications [3, 7, 8].

Conflict of interest

The author declares no conflict of interest.

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