Citation for published version:
Zeidler, A & Crichton, WA 2017, 'Materials under pressure', MRS Bulletin, vol. 42, no. 10, pp. 710-713.
https://doi.org/10.1557/mrs.2017.208

DOI:
10.1557/mrs.2017.208

Publication date:
2017

Document Version
Peer reviewed version

Link to publication

Materials under pressure

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Pressure in manufacturing and life sciences is a key parameter in defining the state of matter. In this special issue of *MRS Bulletin*, we focus on several of the many and diverse domains of advanced materials research where the pressure (or stress) applied is used to alter or otherwise garner information on the material properties. We give an overview of research in which the application of high pressure – often combined with high temperatures and advanced analysis – has led to technological progress in the preparation of superhard materials, in discovering new chemistry for the dense forms of low-Z elements, and in the interplay and mimicking of chemical-induced versus pressure-induced structural and electronic changes to prepare new magnetic and energy materials. In addition, the response of materials such as glasses and perovskites to high stress conditions is discussed, where pressures in the gigapascal regime can easily be achieved in everyday usage. Finally, the structural, dynamical and phase behavior of biological systems is considered.

Keywords: high pressure, densification, hardness, elastic properties.

Introduction

On planet Earth, the pressures can range from 1 bar at the surface, to a few 100s of bar at the bottom of the oceans, to around 360 GPa at the Earth's center (Figure 1). In comparison, the pressure at the center of the sun is estimated to be around 26.5×10^6 GPa. Throughout history, scientists have been motivated to attain ever higher pressures in the laboratory, so as to reproduce and study some of the phenomena seen in real life, and to create novel materials with exciting new properties [1-5]. Here, the applied pressure can be varied almost continuously by more than seven orders of magnitude above ambient pressure, and its influence can have a profound effect on the electronic structure, bonding and coordination environments of atoms, the rates and types of possible reactions, and the microscopic to macroscopic volumetric response and deformation to such loads.

In this way the state of matter can be changed in a controlled way. In addition, advances in instrumentation are enabling completely new regions of phase space to be explored by experiment, while at the same time giving enhanced access to the information that is required to solve materials related issues. What is meant by "high pressure" depends on the field of interest. Pressures can be small at just a few tens of MPa, as in the investigation of biological systems such as the extremophile organisms that live at the bottom of the oceans or the study of protein folding, or, pressures can be in excess of 1 TPa, which are not found naturally on Earth, but are achievable in shock compression experiments that are leading to the discovery of novel states of matter and novel physico-chemical phenomena [6]. The theme of this special issue is 'Materials under pressure'. It presents an overview of recent advances in high pressure experimental methods and instrumentation (such as diamond anvil cells (DACs) [7], multi-anvil presses [8] or the Paris-Edinburgh press [9]; Figure 2) to study matter in materials science, physics, chemistry, engineering and biology.

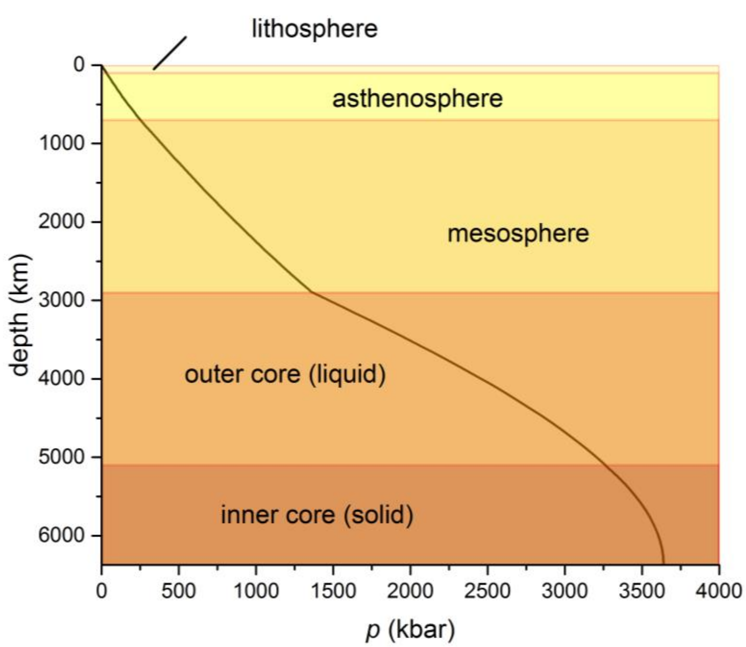

Figure 1: The pressure inside the Earth as a function of depth. The data is take from the Preliminary Reference Earth Model (PREM) of Dziewonski and Anderson[10].

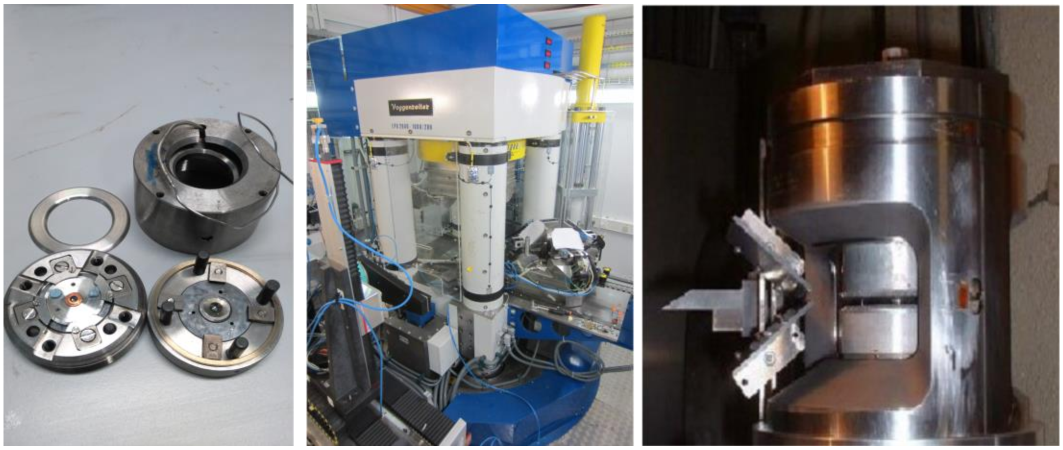

Figure 2 Shows examples different high pressure device types in use at synchrotron and neutron sources; a) a membrane-driven diamond-anvil cell, b) a four-column 20MN large-volume multi-anvil press and c) a VX Paris-Edinburgh press with collimator and shielding for neutron scattering studies.

Superhard Materials

In the first article, Sumiya and Harano report on current progress in the development of ultra-hard materials for abrasives, cutting tools, wire dies, etc.[11] This work extends the discussion of the March 2003 edition of *MRS Bulletin*[12] towards the nanoscale, with illustration of binderless nanopolycrystalline diamond and cBN phases. These synthetic ultra-hard materials surpass the physical properties of microscopic and single-crystal materials through loss of binder and the absence of cleavage and anisotropy [13]. Sumiya and Harano discuss the industrial significance of these materials from the high pressure and temperature sintering processing and their influence on the microstructure as well as their mechanical properties. They also discuss how these tie to the eventual improved application of both nanophase diamond and cBN in high-precision machining in non-ferrous advanced alloys and ceramics and for ferrous materials, respectively [14,15].

Superhigh Pressures

At the extreme pressures occurring deep in planets and stars different, and up to now unknown, chemistries form in extended and dense forms of low-Z compounds. In the second article, Yoo [16] draws from the behavior of ices [17], CO_2 [18,19] and nitrogen [20-22] to illustrate some of the structures that have been discovered and their associated properties. This work opens up the opportunity to make novel compounds with e.g. new piezoelectric, ferromagnetic or superconducting functionality [23-24], or extremely high energy densities. It may prove possible to recover to ambient conditions long-lifetime metastable materials with transformative properties, as is amply illustrated by the existence and super-hard properties of diamond.

Chemistry at High Pressure

Pressure can be used as a method to access and tune structural and electronic configurations not available at atmospheric conditions. Once the desired property is identified, and the structure is determined, an attempt can be made to reproduce this structure using alternative synthesis methods. In their article, Postorino and Malavasi illustrate these effects with two classes of modern technological materials [25].

Firstly, the pressure-induced variation of the properties of hybrid perovskites for solar energy cells (see also *MRS Bulletin*, June 2014 [26]; August 2015 [27]) are illustrated and discussed in parallel with the chemically induced changes that occur by substituting different halides or organic ligands [28-30]. The authors amply illustrate how both the band-gap and carrier lifetime – both critical for solar application – could be influenced by substitution or via substrate selection, thus suggesting new (potentially pressure-influenced) directions of approach to longstanding issues.

The second class of materials are manganites which show exceptional magnetic and electronic functional diversity [31]. They exhibit phenomena that range from high-temperature superconductivity to colossal magnetoresistance.

Postorino and Malavasi demonstrate the wide applicability of the diamond-anvil cell (DAC) to combined measurements of the structure, optical, electronic and magnetic properties of these materials, often made in parallel. With the DAC they are able to influence the many degrees of freedom that affect the above mentioned phenomena; those intrinsic (e.g. chemistry, ionic radii) as well as extrinsic (e.g. temperature, pressure, applied field). These investigations can illustrate rich phase diagrams of manganites [32,33], with possible metallic, insulating, charge-ordered and/or various magnetic phases.

Plastic Deformations

How the elastic moduli, which control fundamental mechanical properties of deformation and rheology, will be affected by pressure is discussed in the article of Carrez and Cordier [34]. The fact that the elastic moduli and pressure scales are of a similar order implies that they will have a significant effect on the bonding, strength and dynamics of materials studied under load. This is further complicated by the presence of defects – point defects, dislocations and grain boundaries - in materials and to what extent these are affected according to the class of material. The authors draw on examples from calculations on the pressure response to defect behavior in bcc metals [35,36], in ionic [37] and covalent systems to illustrate the wide variation possible. They extend this discussion to illustrate the contrasting behavior of two forms of $MgSiO_3$, the perovskite [38] and the post-perovskite [39], which lie on either side of one of the more fundamental of deep Earth transformations.

Glasses under Pressure

Increasing defect density further, in the next article [40]; the inherently disordered nature of glasses makes any investigation into its structural response a complex task. Much ground has, however, been covered in recent years in the characterization of glasses at all length scales [41,42]. The local atomic environments such as the bonding, coordination and angular distribution of adjacent units, and how these are organized on an intermediate scale have been investigated. These have been linked to the macroscopic mechanical bulk responses to increased load or strain [43]. Salmon and Huang discuss the importance of pressure on the ability to control and understand the mechanical properties of a glass. They illustrate that harder, more robust, denser glasses are desirable for scratch resistance, or for changing optical properties, where the power of lenses, or the resolution of a microscope are given by functions of the refractive index, which generally varies with density. As in other materials, glasses can be affected by both mechanical and chemical pressure in order to change the structure and properties of these materials [44-45]. High pressures in the GPa regime are produced at the tip of an indenter, which is used to scratch or deform the surface of the glass [46-47]. Glasses can have inherently long relaxation times. This means that it is possible to recover new materials from high pressure conditions in a densified form which may lead to more fracture resistant materials. Experimental and computational technology can now be used to investigate the response of glasses to tests of these functionalities through a detailed understanding of the structure-property relation of these materials [48-49].

Biological Systems under Pressure

High pressure is also an important parameter in natural systems, with an augmenting interest in biotechnological application. As in inorganic systems, the application of pressure affects reactions, activation barriers and reaction rates; Czeslik *et al.* discuss the complex processes involved and the methods employed for investigating how reactions in biological systems can be affected by the application of hydrostatic pressure, calling on enzymes as example [50]. As enzymes are natural catalysts, they are key to developing more advantageous biotechnologies [51-52]; particularly when pressure can be used to enhance reaction rates when other extrinsic parameters cannot; e,g, when higher temperatures might cause denaturation [53-54]. Other features such as hydrogen bonds will be strengthened, hydrophobic and hydrophilic interactions interrupted, new conformations formed, flexibility in structural conformation tuned, and the overall energetic description of the process will also play a role [55]. The authors show such enzyme activity using stopped flow technology in a well-chosen model system that reveals how pressure could be useful to biotechnological applications [56-57]. The pressures involved in this case are orders of magnitude smaller (in the MPa regime) than in the inorganic systems discussed earlier.

Summary

In summary, pressure can have a dramatic effect on materials' structure and properties and hence it can be used as a means for manipulating and probing materials of technological and biological interest.

Acknowledgements

AZ is supported by a Royal Society – EPSRC Dorothy Hodgkin Research Fellowship.

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