RESEARCH ARTICLE

High Pressure Technology and Its Applications in Materials Science

Guangyu Deng
Shandong University, Jinan, Shandong, 250100, China

Abstract: This paper introduces typical instruments to generate static high pressures were introduced, several representative works in materials science were presented. Matter undergoes changes in physical, chemical, and structural characteristics when subjected to high pressure. Therefore, high pressure is a driving force for new materials, new phenomena, and new effects, and plays an increasingly important role in materials science. High pressure is not only an important means of synthesizing new materials, but also effective in microstructure modulation and performance regulation. It is an important way to develop high-performance materials.

Keywords: High pressure science; materials science; high pressure technique; diamond anvil cell

Citation: Guangyu Deng, 2019. High Pressure Technology and Its Applications in Materials Science. *Advances in Material Science*, 3(1): 1-4. http://doi.org/10.26789/AMS.2019.01.001

1 Introduction

As a physical quantity, pressure refers to the force acting perpendicularly to the surface of an object. The international unit is Newton (N). The pressure is the size of the pressure per unit area, the international unit is Pascal (1Pa=1N/m^2). In actual use, pressure is usually also called pressure, which can be distinguished by unit. In the vast universe, pressure is ubiquitous and changes in a very large range: the pressure generated by the thin hydrogen in interstellar space is 10^{-25}Pa; the pressure in the core of a neutron star is as high as 10^{35}Pa. Taking the earth as an example, the surface pressure of humans' daily life is 1 atmosphere (10^{5}Pa), while the pressure in the center of the earth is about 3.6 million atmospheres.

Conventional material science is usually carried out on a two-dimensional plane composed of temperature and composition. With the addition of the pressure dimension, the entire material world will be greatly enriched. High-pressure science is an emerging discipline that studies the physics, chemistry, mechanics and other behaviors of substances under ultra-high pressures. Its research objects are mainly condensed matter, and the applied pressure is more than tens of thousands of atmospheres. The implementation of high pressure greatly compresses the atomic volume and significantly changes the interactions between atoms within the substance, which can cause changes in the physical and chemical properties of the substance, lead to novel chemical reaction mechanisms, induce structural phase changes of elements and their compounds, and change the earth and planetary materials The rheological properties and so on. High-pressure scientific research therefore plays an important role in promoting many basic disciplines (physics, chemistry, materials science, earth science, etc.). The author briefly introduces several high-voltage generating equipment commonly used in high-voltage science and several applications of high-voltage technology in materials science.

2 High-voltage experimental equipment

There are many types of high pressure generating equipment, which can be divided into dynamic high pressure and static high pressure according to the experimental conditions for providing high pressure. Dynamic high pressure is an instantaneous extremely high pressure of up to millions or even hundreds of millions of atmospheres obtained by using the inertial response characteristics of materials under the action of shock waves driven by detonation, high-pressure gas cannons or lasers; static high pressure is mechanically loaded The method slowly applies a load to the studied material, thereby generating a higher steady-state high pressure (tens of thousands to millions of atmospheres). Although the pressure provided by dynamic high pressure technology is much higher than that of static high pressure technology, it has strict experimental requirements and the pressurization process is short, which cannot be assembled in ordinary laboratories. The static high-pressure equipment is easy to install and use in ordinary laboratories, and the experimental temperature can be set according to the needs, or combined with other experimental detection methods, in situ analysis of changes in materials under high pressure. In the field of materials science, static high pressure technology is increasingly applied to the synthesis and performance research of new materials. Typical static high pressure experimental equipment is based on the pressure provided, mainly six-anvil high pressure apparatus with a large cavity in centimeter size, which can provide a pressure range of 1~10GPa (1GPa is 10,000 atmospheres) ; Two-stage multi-anvil system with millimeter-sized cavity, pressure range of 10~30GPa; diamond anvil cell (DAC) with micron-sized cavity, can provide up to 400GPa Static pressure [1]. For example, take a six-sided top press as an example. Its main body is 6 working cylinders with cemented carbide top hammers on the top. In the high-pressure experiment, the hydraulic system drives the 6 top hammers to move to the center synchronously, and the extrusion is used as pressure transmission. The pyrophyllite block of the medium realizes pressure transmission, so as to obtain the set high pressure in the sample cavity located in the center of the pyrophyllite block. The pressure of the sample chamber of the six-side top press is calibrated in advance by metals such as Bi, Tl, Ba (the resistance of these metals will change suddenly under the corresponding phase change pressure); the temperature of the sample chamber is measured by a thermocouple. Take the CS-IV-D six-sided top press made in China as an example. Its working pressure is 1~6GPa, the working temperature is 300~2300K, and the sample size is above 1cm. The two-stage multi-anvil press can be regarded as an additional set of anvil components in a large six-sided top press. Although the volume of the sample chamber is significantly reduced, the pressure of the chamber is doubled, which can be used for more Synthesize millimeter-sized samples under high pressure. The sample cavity (micron level) of the diamond anvil is sealed by a pair of diamond indenters and gaskets. The sample and the ruby used to calibrate the pressure are placed in the sample cavity filled with the pressure transmission medium, and then the anvil is tightened with a bolt . Due to the large area of the mechanical pressurizing part and the small area of the top end of the diamond indenter, the pressure chamber of the diamond anvil can obtain a high pressure of hundreds of thousands to millions of atmospheres. In recent years, with the improvement of pressure and temperature measurement technology, the application of laser heating technology and the development of various in-situ experimental test methods (electrical conductance/thermal conductance measurement, X-ray diffraction, Raman spectroscopy, synchrotron radiation, etc.), diamond Anvil technology has become a powerful method to study the changes in the structure and properties of substances under extreme pressure conditions.

3 The physical and chemical properties of high pressure

Like temperature and composition, pressure is also an independent thermodynamic parameter that regulates the structure and properties of materials. That is to say, pressure has an effect that cannot be replaced by other means. With the above-mentioned high-pressure generating equipment, materials science research can be carried out under a pressure environment of tens of thousands to millions of atmospheres. Generally speaking, a substance undergoes an average of 5 phase changes per million atmospheres (or 5 new materials appear). Most of these new phases appearing under high pressure have novel physical and chemical properties that the normal pressure phase does not have.

3.1 New materials

Under normal conditions, diamond-structured silicon (d-Si) is the most stable and the most important semiconductor material at this stage, but the inherent indirect band gap of this material makes it incapable of being a next-generation platform for semiconductor technology. Recently, a new allotrope of silicon with a quasi-direct band gap has been synthesized [2]. Experimentally, Strobel et al. first used a two-stage multi-anvil press to prepare a Na_4Si_{24} precursor under a pressure of 10 GPa, and then annealed Na_4Si_{24} in a vacuum environment for a long time to remove the Na atoms in the structure, and finally obtained a kind of orthogonal Structure of Si allotrope (Si_{24},). Si_{24} maintains the advantages of traditional silicon, such as doping potential, structured oxide layer, etc. At the same time, the quasi-direct band gap of the material can significantly improve the optical performance of the material, and its 1.3eV band gap is also very suitable for photovoltaic applications (requires optical band The gap is less than 1.5eV).

3.2 New phenomenon

Na under normal temperature and pressure conditions is an active metal with a body-centered cubic structure, which can be described by a near free electron model.

However, under pressure, the structure of metal Na will undergo multiple phase changes and transform into an optically transparent insulator under a pressure of 200 GPa [3]. Under such a high pressure, the volume of the sample is compressed to 1/5, the crystal structure changes from a body-centered cubic structure to a double hexagonal close-packed structure (Na-hP4,), the distance between Na atoms is significantly reduced, and pd doping occurs in valence electrons. The transformation leads to a strong localization of the electronics, which turns into an insulator.

3.3 New effects

Hydrogen is the lightest element in the periodic table, and monoatomic hydrogen is also the most common substance in the universe. In 1935, Wigner et al. [4] predicted that molecular hydrogen would metallize under high pressure; in 1968, Ashcroft [5] further predicted the room temperature superconductivity of hydrogen under high pressure. The metallization and superconductivity of hydrogen have always been regarded as the Holy Grail of high-voltage science, stimulating human research enthusiasm. Existing studies have shown that at least a high pressure above 4 million atmospheres is required to achieve hydrogen metallization, and a higher pressure is required to achieve superconductivity [6]. This is still a challenging problem from the perspective of high-pressure technology [7]. Fortunately, in recent years, breakthroughs have been made in the research on the high-voltage superconductivity of hydrogen-rich compounds. For example, the superconducting transition temperature of the cubic structure of LaH10 at a pressure of 170GPa is 250K, which is close to room temperature. These results also provide confidence and new impetus for chasing the holy grail of hydrogen metallization and superconductivity.

4 Application of high pressure technology in materials science

The application of high-pressure technology in the field of materials science has produced fruitful results. Pressure is therefore the source of discovering new materials, new phenomena, and new effects. Pressure can also control the microstructure of materials and significantly improve material properties, which is an important way to develop high-performance materials. Take diamond as an example. The hardness of natural diamond is about 100 GPa, which is the key material for making diamond counter anvils. However, the fracture toughness of diamond is not high, and it is prone to cleavage and fragmentation during use, which severely limits the ultimate pressure and service life of the diamond cavity on the anvil. Huang et al. used an onion-structured carbon precursor to synthesize a diamond block with an ultrafine nano-twin structure through high temperature and high pressure (20GPa, 2000°C) phase transformation. A high-density twin substructure is formed inside the nanocrystals in the bulk material, and the average twin thickness is as low as 5nm. The performance of the material has reached an unprecedented level: the hardness is as high as 200GPa, which is twice the hardness of natural diamond, realizing the human dream of synthesizing artificial materials harder than natural diamond; fracture toughness is 10~15MPa•m$^{1/2}$, It is equivalent to commercial cemented carbide. By optimizing the experimental temperature and pressure conditions (15GPa, 2000℃), the microstructure of nano twin diamond can be further controlled, and a diamond composite material with multi-level structure characteristics can be prepared: as the scale increases, coherent Diamond polytype (thickness of several to ten atomic layers), interwoven cubic structure diamond nano twins (thickness of several nanometers) and interlocked diamond nanoparticles (tens of nanometers) are sequentially assembled in stages. This multi-level structure of nano-twinned diamond composite materials endows the material with extremely high hardness and toughness. While maintaining the hardness of 200GPa, the fracture toughness of nano-twinned diamond is increased again to 26.6MPa•m$^{1/2}$, which is about 5 times the toughness of synthetic diamond, which is higher than that of magnesium alloy and comparable to aluminum alloy.

5 Conclusion

The extremely hard and tough nano-twinned diamond and its composite materials are particularly suitable for ultra-precision machining and are expected to bring about technological changes in the mechanical processing industry. This type of material is also suitable for making diamond counter anvils. Using ultra-high hardness nano twin diamonds as an anvil, it is possible to achieve static high pressures above 1000 GPa, providing necessary experimental conditions for uncovering scientific mysteries such as metal hydrogen. Broadening the range of experimental pressure for humans to explore new materials, new phenomena, and new effects is expected to bring about breakthrough technological changes in the research fields of earth sciences and high-pressure sciences.

References

[1] Li B,Ji C,Yang W G,et al. Diamond anvil cell behavior up to 4 mbar[J]. Proceedings of the National Academy of Sciences of the United States of America,2018(08):1713-1717.

[2] Kim D Y,Stefanoski S,Kurakevych,et al. Synthesis of

an open-framework allotrope of silicon[J]. Nat Mater, 2015(14):169-173.

[3] Ma Y,Eremets M,Oganov A,et al. Transparent dense sodium[J]. Nature,2009(7235):182-185

[4] Wigner E,Huntington H B. On the possibility of a metallic modification of hydrogen[J]. The Journal of Chemical Physics, 1935(12):764-770.

[5] Ashcroft N W. Metallic hydrogen: A high-temperature superconductor? [J]. Phys Rev Lett,1968(21):1748-1749.

[6] Pickard C J,Errea I,Eremets M I. Superconducting hydrides under pressure[J].Annual Review of Condensed Matter Physics,2020(11):57-76.

[7] Loubeyre P,Occelli F,Dumas P. Synchrotron infrared spectroscopic evidence of the probable transition to metal hydrogen[J]. Nature,2020(7792):631-635.