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Recent advances in high-pressure science and technology

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Abstract

Recently we are witnessing the boom of high-pressure science and technology from a small niche field to becoming a major dimension in physical sciences. One of the most important technological advances is the integration of synchrotron nanotechnology with the minute samples at ultrahigh pressures. Applications of high pressure have greatly enhanced our understanding of the electronic, phonon, and doping effects on the newly emerged graphene and related 2D layered materials. High pressure has created exotic stoichiometry even in common Group 17, 15, and 14 compounds and drastically altered the basic σ and π bonding of organic compounds. Differential pressure measurements enable us to study the rheology and flow of mantle minerals in solid state, thus quantitatively constraining the geodynamics. They also introduce a new approach to understand defect and plastic deformations of nano particles. These examples open new frontiers of high-pressure research.

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1. Introduction

High-pressure research has been advancing rapidly during the last decades, thanks to the concerted development of various pressure devices and probing technology. The migration of numerous dedicated synchrotron techniques to high-pressure research has greatly impacted fundamental physics, chemistry, Earth, and materials sciences.

Recent discoveries in high-pressure condensed matter physics include the metallization of hydrogen, quantum criticality, high T_c superconductors, polyamorphism, and exotic metals. High pressure can dramatically decrease the atomic volume and increase the electronic density of the reactants, which will result in novel and special chemical reactivity, kinetics and the reaction mechanisms. Particularly noticeable are the pressure induced transitions in elements, molecular compounds, ionic compounds, and high pressure chemistry reaction assisted by photochemistry and electrochemistry. The rheological properties of Earth and planetary materials can now be well characterized with controlled strain rate at high pressures using synchrotron X-ray diffraction and imaging. The dislocation and grain rotation of nanomaterials can be quantitatively studied with pressure tuning.

The impact of the pressure dimension has expanded rapidly to cover a wide domain of physical sciences. It will not be possible to have a comprehensive coverage of the entire frontiers in this article. Instead, we will focus on the advances of several selected areas of great potentials, and present short summaries, highlights, and recent developments. Moreover, the subjects will be limited mostly to static compressions.

2. High-pressure synchrotron X-ray probes

High pressure is a technology dictated science. Over the century-long development of high-pressure technology, record

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pressures doubling that at the center of the Earth [1] can be reached with a minute amount of sample. Synchrotron developments have been one of the major driving forces for the recent breakout of high pressure activities [2]. By taking advantage of the third generation synchrotron sources and fast advanced X-ray optics development, high pressure community has benefited from various techniques to a new level of high pressure studies: like the high brilliance for ultra small focused beam [3], tunability for spectroscopy and resonant scattering [4], circular and linear polarization for magnetic study [5], high energy resolution inelastic scattering for dynamical properties [6], coherence imaging for ultra-sensitive phase contrast for even very light materials at tens of nanometer scale [7], high energy scattering for disordered system, amorphous and liquid phases [8], etc. Traditional high-pressure study mainly focused on the static study, the time-resolved techniques will allow us to study material behavior far from equilibrium and have snap shot during the dynamic process. It is the golden time for integrating these advanced techniques coherently to solve the real world complicated system and understand the materials behavior under extreme environment from all aspects to achieve ground-breaking results. Here we focus on a few highlight works with these advanced probes.

2.1. Local ordering from sub-nanometer resolution with high-energy X-ray diffraction

Under high pressure, material usually consists of highly deformed pieces and turns to very fine crystallites, which causes the severe broadening of X-ray powder diffraction peaks. Although Scherrer equation can be used to de-convolute the strain and particle size effect from the diffraction peak width vs. diffraction angle, it is often hard to distinguish the heavy deformation of nanoparticle from the amorphous states. Atomic resolution transmission electron microscopy has been used as the major tool to probe the microstructure with resolution at sub-nanometer and even sub-angstrom scale from direct high resolution imaging technique. High-energy X-ray diffraction from the other end provides wider Q-coverage (reciprocal space) diffraction information, and upon the Fourier transformation, one can obtain the real space pair distribution function (PDF) distribution at atomic bonding distances. For nano- and amorphous-materials research under high pressure, the high energy PDF study would provide a unique characteristic tool to understand the deformation mechanism and structure stability at atomic scale. For the case of nano-sized Y_2O_3 particles, there is a critical size effect discovered with the PDF tools [9], where 16 nm Y_2O_3 shows totally different structure stability and phase transition route comparing to 21 nm Y_2O_3 particle, while the latter one behaves in the same way as bulk materials. Ta_2O_5 has a unique crystal structure with a very long a lattice comparing to the other axes ($a = 43.997$ Å, $b = 3.894$ Å, $c = 6.209$ Å with a Pmm2 space group) [10]. Looking at the bonding structure along a, there are several weak bonded connections. High energy PDF was applied to the in-situ high pressure structure study, and clear local bonding breakage can be seen at different pressure stage (Fig. 1). For comparing with the traditional atomic resolution TEM characterization, samples recovered from different pressure stages were checked with TEM, and the clear local order/disorder atomic re-arrangement can be seen which matches the PDF study very well [10], in which combining the traditional TEM probe, high energy PDF demonstrates the super powerful capability for the in-situ local bonding (sub nanometer) order/disorder characterization.

2.2. Nanoscale deformation imaging with the coherent scattering probe

The evolution of morphology and internal strain under high pressure fundamentally alters the physical property, structural stability, phase transition and deformation mechanism of materials. Until now, only averaged strain distributions have been studied. To improve our fundamental understanding of the deformation mechanism, we need to probe individual nano grains under extreme conditions. For doing so, a much higher spatial resolution probe is required. The Bragg coherent X-ray diffraction imaging (CXDI) technique is a promising tool to probe the internal strain distribution and grain shape during the plastic/elastic deformation of individual nanometer-sized single crystals. Coherence diffraction can be realized by setting an entrance slit smaller than the transverse coherence length and an X-ray sensitive area detector at far field to catch the Fourier scattering with high resolution. The third-generation sources of synchrotron radiation using undulators and the upcoming multi-bend Achromat lattice upgrade for major large synchrotron sources have provided a great source to ensure coherence with a practical flux level to conduct experiment. As the coherent X-rays pass through a distorted crystal, both the scattering intensity and phase will be affected. Bragg CXDI operates by inverting three-dimensional (3D) diffraction patterns in the vicinity of Bragg peaks to real-space images using phase retrieval algorithms [11]. In the resulting images, the reconstructed magnitude represents the electron density of the crystal, while the obtained phases are attributed to lattice distortions projected onto the Bragg direction.

The typical experimental setup is shown in Fig. 2(a). A coherent X-ray beam illuminates the sample in a diamond anvil cell (DAC), where the studied crystal is aligned to the rotation center to allow the three dimensional phase retrieval. An X-ray sensitive area detector is placed at far field to catch the Bragg scattering intensity. With a phase retrieval algorithm, the reciprocal space diffraction information is Fourier transformed to the real space with multiple iterations till convergence of both amplitude and phase is reached. The amplitude is proportional to the electron density, while the phase part is used to characterize the strain field. This has been well used to construct the shape and internal strain distribution after the plastic deformation under high pressure at different pressure environment in a 400 nm sized gold particle [12]. Fig. 2(b) shows the shape and strain evolution in this nano-gold particle under pressure up to 6.4 GPa. One can see the shape evolution at various pressure which corresponds to the single crystal rheology as activated dislocations are created