Reaserch Organization (KEK), Tsukuba 305-0801, Japan., E-mail：hirao@spring8.or.jp

High pressure can produce a very steep increase of the chemical potential of hydrogen, resulting in a drastic enhancement of the solubility in metal. A number of transition metal hydrides have been synthesized under high-pressure conditions. As far as the platinum group metals are concerned, these metals have been generally known as highly active catalysts in metal-hydrogen systems. There has been experimentally no observation of platinum metal hydrides, except for palladium and rhodium hydrides. A theoritical calculation predicts formation of platinum metal hydrides with high concentration of hydrogen at high pressure. We investigated iridium-, platinum-, and gold-hydrogen systems at high pressure to synthesize metal hydrides. In platinum-hydrogen system, a pressure-induced structural phase transition of face-center-cubic phase into hexagonal-close-packing + tetragonal phases was observed at 24-25 GPa by in situ X-ray study. The volumes of new phases are likely to propose the formation of platinum hydrides. In other systems, no formation of metal hydrides was observed up to 30 and 40 GPa, respectively.

Keywords: diamond anvil cells, high-pressure synthesis, metallic hydride

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Pressure-induced structural transition in rare-earth metal hydrides

Akihiko Machida[1], Tetsu Watanuki[1], Ayako Ohmura[1], Katsutoshi Aoki[1], Kenichi Takemura[2]
[1]Japan Atomic Energy Agency, Synchrotron Radiation Research Center, 1-1-1 Kouto, Sayo-cho, Sayo-gun, Hyogo, 679-5148, Japan, [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki, 305-0044, Japan, E-mail：machida@spring8.or.jp

Pressure induced structural transitions of rare-earth metal hydrides have been investigated under hydrostatic pressure at room temperature. Tri-hydride, YH_3, exhibits a hexagonal metal lattice containing three hydrogen atoms per metal atom in the interstitial spaces: two hydrogen atoms at the tetrahedral sites and one hydrogen atom near the Y metal plane in the octahedral sites. To study high-pressure structural properties, we performed synchrotron radiation x-ray diffraction experiments by using a diffractometer for diamond anvil cells installed at the BL22XU beamline in SPring-8. We observed the pressure-induced structural transformation from the hexagonal metal lattice into a face-centered cubic (fcc) one through an intermediate state, which appears in the wide pressure span of 12-22 GPa. The obtained x-ray diffraction patterns in the intermediate state are represented by long-period rhombohedral structures, e.g. 27R, of the yttrium metal lattice. These long-period structures are interpreted in terms of the periodic arrangements of hexagonal-type (ABA or h-type) and fcc-type (ABC or k-type) stacking layers of the yttrium metals. For example, 27R structure described as (hhhhkkk)3 by Jagodzinski notation is one of plausible models for 14.0-GPa structure. These long-period structures gradually transform toward the fcc metal lattice with successively increasing in the fcc-type component in a unit cell upon compression. Such structural transition is considered to be characteristic for rare-earth metal hydrides and should be interpreted in terms of the hydrogen-hydrogen interactions and hydrogen-metal bonding.

Keywords: high-pressure structure determination, high-pressure X-ray diffraction, hydride structure

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Toward fully automated high pressure beamlines : Recent developments at beamline ID27, ESRF

Mohamed Mezouar, Jean-Philippe Perrillat, Gaston Garbarino, Wilson A. Crichton, Stany Bauchau, Holger Witsch
ESRF, BP 220, Grenoble, Isere, 38000, France, E-mail：mezouar@esrf.fr

The automatic collection of high quality X-ray diffraction data at high pressure and high or low temperatures is a new and very challenging method. Indeed, it involves the development of specific pressure and temperature devices that can easily be interfaced to the beamline control computer in order to achieve a sequential series of command at a given pressure and temperature. This sequential series includes the automatic sample alignment, pressure and temperature measurements and XRD data collection. We present a recent development at beamline ID27 which allows the fully automated collection of high pressure XRD data in a membrane type diamond anvil cell. The potential of this new development is illustrated on a school case: the equation of state of platinum.

Keywords: X-ray diffraction, high pressure, automation

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High pressure single-crystal neutron diffraction of squaric acid

Craig L Bull, Malcolm Guthrie, Richard J Nelmes, John S Loveday, Kazuki Komatsu
University of Edinburgh, School of Physics and Centre for Science at Extreme Conditions, JCMB, The Kings Builidngs, Mayfield Road, Edinburgh, Mid Lothian, EH9 3JZ, UK, E-mail：c.bull@rl.ac.uk

Although powerful in many cases, the 1-d character of a powder diffraction pattern inevitably leads to loss of information due to peak overlap. Hence, detailed structural studies such as measurement of anisotropic thermal motion and multi-site disorder sometimes require the full 3-d information extracted from single-crystal data. It is currently possible to determine single-crystal diffraction patterns from micron-sized samples up to a pressure of 1 Mbar using x-ray synchrotron sources. However, form-factor effects limit the resolution of the information that can be obtained by this technique on thermal motion and disorder, particularly in the lighter elements. Neutron diffraction is the technique of choice for extracting such information from light elements, although the relatively low fluxes available mean that a sample volume in excess of 1mm3 is required. As a consequence, the devices used to generate pressures typically exploit significantly different approaches from those used at synchrotrons. To this end, we have been developing new anvil geometries and cells which allow us to collect high-resolution single-crystal neutron diffraction data up to a pressure of 8GPa. We present the results of a study in which we have used these techniques to follow a proposed hydrogen-bond centring transition previously proposed in squaric acid at ~3GPa. Just beyond this pressure, we have seen no evidence for hydrogen-bond centring but observe an extended hydrogen distribution between the oxygen atoms. Neutron diffraction data have been collected using time-of-flight techniques at the ISIS Facility, and monochromatic techniques at the Institut Laue-Langevin. The results will be presented, including details of data reduction and the techniques used to collect the new data.

Keywords: high pressure, single crystal, neutron diffraction