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High-pressure equation of state for gold with a He-pressure medium

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High-pressure powder x-ray diffraction experiments have been done on gold with a He-pressure medium up to 130 GPa at room temperature. We have conducted independent experiments at the Photon Factory and ESRF in order to check any systematic experimental errors. Effects of uniaxial stress were evident, in both experiments, at pressures higher than 30 GPa in ruby luminescence spectra and x-ray diffraction patterns. This demonstrates the pressure limit of solid He as a purely hydrostatic pressure medium. The stress states were analyzed with the use of the gamma-plots [1]. The uniaxial stress components were calculated by assuming the elastic moduli of gold under high pressure, and were found to range from - 0.6 GPa to + 0.9 GPa, depending on the experimental conditions. The difference of the stress states is the likely cause for the discrepancy in the equation of state parameters of gold previously reported [2, 3]. By properly correcting the effects of uniaxial stress components on the measured lattice parameter, the equation of state of gold is now well established.

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Keywords: diamond anvil high-pressure apparatus, equations of state, high-pressure X-ray diffraction

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Infrared spectroscopy of aluminum trihydride α-AlH_3 under high pressure

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Aluminum trihydride (AlH_3) has seven crystalline polymorphs (α-, α'-, β-, γ-, δ-, ε-, ζ-) composed of the octahedral AlH_6-unit. The α-phase (α-AlH_3, space group *R*-3*c*: *a* = 4.499 Å and *c* = 11.804 Å) is reported to be most stable and insulator with an interatomic Al-H distance (r_{Al-H}~1.72 Å) between the values expected for covalent bonding (~1.5 Å) and ionic one (~2.0 Å). α-AlH_3 has been studied as a candidate for the hydrogen storage material owing to its high gravimetric hydrogen density (10.1 mass%) and low dehydriding temperature (370-470K). However, there are still some unresolved matters regarding recyclability because it's necessary to apply ~ GPa pressure for re-hydrogenation of aluminum, namely Al-H bond formation. So, to evaluate the bonding properties of α-AlH_3, we performed the high-pressure infrared spectroscopy of α-AlH_3 using diamond anvil cell. α-AlH_3 was synthesized by the metathesis reaction of $LiAlH_4$ and $AlCl_3$ in diethyl ether followed by a desolvation process. The specimen with ~1 μm thick is loaded in the rhenium gasket with KBr which is pressure transmitting medium. Infrared vibrational absorption spectra are measured for α-AlH_3 with increasing pressure between 1.9 and 60 GPa at ambient temperature. The peak frequency shifts monotonically and no notable spectral changes are observed up to 60 GPa, which agrees with recent x-ray diffraction measurement performed by Goncharenko *et al*., while the sample gradually get black beyond 45 GPa. The mode Gruneisen parameter γ for the Al-H bond stretching-mode is derived to be 0.37 from the observed peak shifts and the bulk modulus reported by Baranowski *et al*. The value is almost same as those for alanates, $LiAlH_4$ and $NaAlH_4$, which are typical covalent-bonding materials.

Keywords: high-pressure research, infrared spectroscopy, hydrogen storage

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X-ray study for new filled skutterudite $DyRu_4P_{12}$ at ambient and high pressures

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Ternary metal pnictides LnT_4X_{12} (Ln = lanthanide, actinide; T = transition metal; X = pnicogen) crystallize with a filled skutterudite-type structure. This structure is cubic, space group Im-3, *Z* = 2. Ln atoms locate at (000) and (1/2 1/2 1/2) of body-centered cubic structure. T atoms are in the center of a distorted octahedral environment of six X atoms. The skutterudite compounds show interesting electrical and magnetic properties at low temperatures. New filled skutterudite with heavy lanthanide $DyRu_4P_{12}$ have been prepared at high temperatures and high pressures. We have studied powder x-ray diffraction of $DyRu_4P_{12}$ with synchrotron radiation at ambient pressure and high pressures. The skutterudite compounds were prepared by reaction of each metal and red phosphorus or powders at high pressure and high temperature. Using synchrotron radiation, powder x-ray diffraction patterns of these compounds were measured with a diamond-anvil cell and an imaging plate at high pressures. A 4:1 methanol-ethanol solution was used as pressure medium. The pressure in the diamond-cell was measured before and after each exposure based on the shifts of the ruby R1 fluorescence lines. The crystal structure of $DyRu_4P_{12}$ was refined by the Rietveld analysis of powder x-ray diffraction data at ambient pressure. The lattice constant of this compound is 8.0294 Å. The positional parameters, bond distances and bond angles are obtained. Powder x-ray diffraction patterns of $DyRu_4P_{12}$ were measured with synchrotron radiation at high pressures. The cell volume of this skutterudite monotonically decreases with increasing pressure up to about 10 GPa. New diffraction lines do not appear up to 10 GPa although the diffraction lines shift and the width broadens with increasing pressure.

Keywords: high pressure, synchroton radiation, powder X-ray diffraction