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High pressure compounds in xenon-hydrogen mixtures

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The study of binary mixtures of atomic (He, Ar, Xe, etc.) and diatomic (N_2, O_2, H_2, etc.) molecular solids is relevant for a better understanding of the interior of the giant planets. It has lead to the discovery of a new type of compound – the van der Waals (vdW) compound – and provides essential information on the interactions among simple molecules.

It was long believed that group 18 elements were inert and unreactive and could not form compounds. A new chemistry field started in 1962, when the first noble gas compound, xenon hexafluoroplatinate, was synthesised [1]. Since then, many compounds have been created combining noble gases with other chemical elements [2].

Here we present a study of vdW compound formation in the xenon-hydrogen system under high pressure. We have studied several compositions (between 7% and 15% vol Xe) to map the binary phase diagram. Complex phase behaviour as a function of composition and pressure was observed with the formation of different stoichiometric phases.

These novel Xe-H_2 compounds have been characterized by single-crystal and powder x-ray diffraction at beamline I15 of Diamond Light Source. We find three separate phases with orthorhombic, hexagonal and rhombohedral structures as function of pressure and composition. These novel structures will be presented in relation to other rare gas-hydrogen compounds, in particular $Ar(H_2)_2$ [3], $Kr(H_2)_4$ [4], and the previously reported $Xe(H_2)_8$ [5].

A rare gas hydrogen system not only offers the possibility of the discovery of unusual stoichiometric compounds, but also allows the study of the hydrogen molecule in a modified environment compared to pure H_2 solid. The study of the detailed intra-molecular response of H_2 to compression can give insight into new pathways to hydrogen metallization. This has been suggested for the $Ar(H_2)_2$ compound [3]. In the Ar-H system the H_2 vibron is seen to increase continuously under pressure. In contrast our Raman spectroscopic measurements on rhombohedral $Xe(H_2)_8$ show shifted vibron frequencies relative to the pure (bulk) H-H stretching mode which soften with pressure and appear to cross the pressure-frequency trajectory of the pure H_2 vibron around 50 GPa.

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Neutron diffraction study on the pressure-induced cubic-tetragonal structural distortion in LaD_2 using total scattering spectrometer NOVA

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Rare-earth metals absorb large amount of hydrogen to form di and trihydrides. For a dihydride LaH_2, in which hydrogen atoms are accomodated in the tetrahedral interstitial sites of the host fcc metal lattice alone and the octahedral sites remain empty, we found a pressure-induced phase separation by synchrotron radiation X-ray diffraction [1]. We also found a lattice distortion from the cubic to a tetragonal one before the phase separation. X-ray diffraction measurements, however, provided no information on the hydrogen positions and occupancies in the metal lattice. They are crutial for undestanding the origin of the lattice distortion and hence the mechanism of the phase separation.

High-pressure neutron diffraction experiments were performed for LaD_2 with a total scattering spectrometer NOVA constracted at J-PARC [2]. Rietveld analysis of an ambient pressure profile of a powder sample yielded a lattice constant a=5.652 (2) Å and hydrogen occupancies 0.94(4) at T-site and 0.09(6) at O-site. In the high pressure experiments, we used a Paris-Edinburgh cell [3]. High pressures up to 10 GPa and above were genarated with single toroid anvils made of tungsten carbide and double toroid anvils of sintered diamond, respectively. LaD_2 powder was encapsulated in a gasket made of TiZr null alloy together with a pressure medium of deuterated methanol-ethanol 4:1 mixture. We obtained diffraction profiles at ten pressure conditions from 0.1 to 17GPa.

The fcc lattice of LaD_2 began distortion to a tetragonal lattice around 7GPa. The peak splitting arising from the tetragonal distortion increased in magnitude on further compression to the phase separation pressure of 11 GPa. A similar lattice distortion has been reported for superstoichiometric $LaH_{2+\delta}$, in which excess hydrogen atoms occupy the O-sites to make the cubic lattice distorted [4]. Partial transfer of the T-site D atoms into the O-sites in LaD_2 is one possible cause for the distortion. Refinement of the diffraction profiles measured for the tetragonal phase at several pressure points are carrying out now. The microscopic mechanism of the cubic-tetragonal structural trasition and the following phase separation will be discussed on the basis of the refined structural parameters.

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High pressure structure and magnetism of one 1-D molecular magnetic material

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Molecular magnetic materials(MMM) have been attracted much attention for increasing demands on smaller size magnetic memory devices and interest in the interpretation of the mechanism for complicated magnetic interactions. Many studies focus on investigating the magnetic coupling mechanism and the magneto -structural correlation. Many methods can be used to control magnetic property.