

Lattice Compression of Lithium Hydride up to 200 GPa

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Lithium Hydride (LiH) is a quantum crystal composing of the lightest ionic elements, which crystallize in the rock-salt structure typical for ionic compounds. The outer-shell electron of Li may fully transfer to H atom to form Li^+ and H^- ions both having two electrons in the 1s orbitals. The ion radii of Li^+ and H^- system are quite different even though the ions have the same electron configuration ($1s^2$): 0.15 nm for H^- and 0.06 nm for Li^+ . Applying pressure would make redistribution of the electron charge as a result of electro static repulsion between the electrons approximately localized around the ions. Theoretical results have suggested slight presence of covalent bonding nature and strong phonon-electron coupling. Insulator-semimetal transition has also been predicted at pressures above 200 GPa with transformation from NaCl(B1) to CsCl(B2) structure [1]. The compression data have been obtained by single crystal diffraction with white x-ray beam technique for LiH and LiD up to 37 GPa and 94 GPa, respectively [2].

We have performed powder diffraction measurement with a monochromatized x-ray at pressures beyond 100 GPa at BL10XU/SPring-8. The maximum pressure currently reached was 202 GPa. The transparency of sample against a back-illumination under microscopic observation have been still clear. No phase transition was observed, and no indications of insulator-metal transition was obtained. The unit-cell volume compression data were in good agreement with the previous experimental work at low pressure range, but it become somewhat incompressible from theoretical calculation at high pressure range (<120 GPa). The lattice constant at 202 GPa was compressed to 0.29 nm (70 % from atmospheric pressure), which have been already shorter than the H^- ion diameter of the ambient value.

Another experiment was made under hydrostatic condition using He pressure-transmitting medium. The angle dispersive measurement enables us to measure diffraction intensity much precisely and hence analyze charge distribution. Four or five homogeneous powder rings were observed, providing integrated intensities available for intensity analysis. The intensity ratio of 111 to 200 reflection decreases slightly but significantly during the pressure loading up to 48 GPa (the lattice constant is compressed to 81 % of the ambient value). This fact suggests that the relation between H^- and Li^+ atomic scattering factor was changed under pressure. The electron around H^- seems to be contracted by compression.

References

1. F.Perrot, Phys. stat. sol. 77 (b), 517, 1976.
2. P.Loubeyre et al, Physical Review B.57, 10403, 1998.