

Accurate structures of diamond under high- pressure and temperature.

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Carbon has attracted wide attention owing to the main component of organics and their several functional allotrope, graphite, graphene, fullerene, and diamond. Diamond is the first structurally characterized material by L. Bragg. We have measured accurate powder diffraction data of diamond at the third-generation synchrotron X-ray source, SPring-8 and PETRA-. We determined accurate charge densities by maximum entropy method (MEM) and multipole refinement from the data [1,2]. We also observed the core deformation of carbon atom from the charge density [3]. These studies confirm that powder diffraction data of diamond is suitable for accurate structural study. The fact suggests that the response of electron distribution under external fields such as temperature and pressure can be precisely revealed by using the powder data of diamond. In this study, we have investigated the temperature and pressure dependence of charge density for diamond from powder data at SPring-8.

Multi-temperature synchrotron powder diffraction data were collected at BL02B2 beamline, SPring-8. The data were measured at 30-800 K using a wave length 0.32905 Å. We have observed bragg reflection at 2.57 Å⁻¹. High pressure powder diffraction experiments using a diamond anvil cell (DAC) were carried out at BL02B1, SPring-8. We measured high pressure powder data up to 3.58 GPa using a wave length 35 keV. We have observed temperature dependence of accurate charge densities of Diamond at 300, 600 and 800K. The covalent bonding in diamond was clearly recognized and was consistent with the previous studies. We also observed that relative intensities of low order reflections, such as 111 and 220, are changed with increasing pressure.

[1] E. Nishibori et al., Acta Cryst. A63, 43-52, 2007.

[2] H. Svendsen et al., Acta Cryst. A66, 458-469, 2010.

[3] N. Bindzus et al., Acta Cryst. A70., 38-48, 2014.

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