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High resolution charge density of metal hexaborides.

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Continuous development of X-ray diffraction instruments enable us to routinely perform charge density study using Laboratory source X-ray. An X-ray at synchrotron radiation facility should show clear advantages to that of Laboratory source. High reciprocal resolution data measured at large 3rd generation synchrotron facilities, such as SPring-8, Petra-III, ESRF and APS, have great advantages to measure such high reciprocal resolution data. It is normally very difficult to measure high reciprocal resolution data with d 0.22 Å reciprocal resolution data measured at SPring-8 [3].

Metal hexaborides MB6, where M is alkaline earth or rare earth metal, exhibit metallic and semiconductor properties by changing the M ion. We investigated the charge densities of divalent and trivalent metal hexaborides, semiconducting BaB6 and metallic LaB6 using the d>0.22 Å ultra-high resolution synchrotron radiation X-ray diffraction data by a multipole refinement and a maximum entropy method. The strong inter-octahedral and relatively weak intra-octahedral boron-boron bonds were observed in the charge densities. A difference of valence charge densities between LaB6 and BaB6 was calculated to reveal a small difference between isostructural metal and semiconductor. The weak electron lobes distributed around the inter B6 octahedral bond were observed in the difference density. We found the electron lobes are the conductiveelectrons in LaB6 from the comparison with the theoretical charge density.

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