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 conductive electrons in LaB₆ from the comparison with the theoretical charge density.


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