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 \( d > 0.22 \text{ Å} \) reciprocal resolution data measured at SPring-8 [3]. Metal hexaborides \( \text{MB}_6 \), 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 \( \text{BaB}_6 \) and metallic \( \text{LaB}_6 \) using the \( d > 0.22 \text{ Å} \) 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 \( \text{LaB}_6 \) and \( \text{BaB}_6 \) was calculated to reveal a small difference between isostructural metal and semiconductor. The weak electron lobes distributed around the inter \( \text{B}_6 \) octahedral bond were observed in the difference density. We found the electron lobes are the conductive electrons in \( \text{LaB}_6 \) from the comparison with the theoretical charge density.


Keywords: Electron charge density; synchrotron powder X-ray diffraction; metal hexaborides