Electron Density of $ScRh_3B_x$: Relation of the Electron Density to the Hardness

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$ScRh_3B_x$(x=0.0-1.0) has been investigated recently as an ultra-hard material. Crystal structure refinements and electron density analyses of this material were carried out by synchrotron X-ray powder diffraction. The powder diffraction data were collected using Multi-Detector System powder diffractometer at the BL-4B2 experimental station of the Photon Factory. The crystal structure refinements were performed using the Rietveld method and the electron density maps were calculated with the Maximum Entropy Method (MEM). The results of the refinements show that the crystal structure of $ScRh_3B_x$ is cubic with Pm3m space group, which has same atomic arrangement with perovskite structure. The lattice constant increases linearly according to the increase of B amount. In the electron density maps obtained by MEM analysis, electron density raises are obviously observed between B and Rh atoms. The rises of electron density show the existence of covalent bond between B and Rh atom. In spite of the liner increase of lattice constant according to the increase of B amount, the hardness of this series of compounds have a minimum between 0.4 and 0.7 of B contents. This change of hardness is supposed to be related to the amounts of the covalent bond in the crystal structure. The bond character of this series of compounds is also discussed based on the results of electron density analyses.

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