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Band structure, density of states, and crystal chemistry of $ZrGa_2$ and $ZrGa_3$ single crystals

Abstract

Using FP-LAPW Method we have performed calculations of the band structure of the $ZrGa_2$ and $ZrGa_3$ crystals. The all-electron full potential linearized augmented plane wave method was used to solve the Kohn Sham DFT equations. We have explored different approximations using three kinds of exchange-correlation potentials on the electronic structure and we concluded that there is insignificant influence on the band structure and the density of states. It is clear that there exists a difference in the band dispersion with one move from $ZrGa_2$ to $ZrGa_3$ that is attributed to the fact that $ZrGa_2$ has four formula per unit cell (Z = 4) while $ZrGa_3$ has two formula per unit cell (Z = 2). Despite some similarity in the crystallochemistry of $ZrGa_2$ to $ZrGa_3$ some differences are observed in the band structure dispersion. There is a strong hybridization between the states. The interaction of charges between Zr and Ga atoms is due to the strong hybridization, and the covalent bond arises due to the degree of hybridization. Hence, there is a strong covalent bonding between these atoms. We have obtained a space electron charge density distribution in the average unit cell by calculations of the electron charge density distribution. The space electronic charge density contour distribution is illustrated in (1 0 0) and (1 1 0) planes.

Keywords: Inorganic materials, Crystal growth, Electronic band structure, X-ray diffraction