Poster Presentation

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Structural chemistry of indium doped Bi_2Se_3

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Bi2Se3 and its solid solution have attracted enormous interest because of their intricate crystal structures, interesting electronic structures and fascinating physical properties. Alloys of Bi2Se3 show outstanding thermoelectric properties. Bi2Se3 adopts a hexagonal layered structure (R-3m (166), a = 4.140798 Å, c = 28.64232 Å) consisting of quintuple layers of Se-Bi-Se-Bi-Se, which are held together by weak van der Waals interactions.

The α-polymorph of In2Se3 is isostructural to Bi2Se3. According to the previous reports, at room temperature In2Se3 can crystallise as several polymorphs depending on the synthetic conditions. The α-polymorph can be stabilised by substitution of bismuth atom in In2Se3.

In this investigation, the effect of In substitution on crystal structure, electronic structure and the thermoelectric properties of Bi2Se3 have been studied. Herein, we will present the changes in property measurements as well as structure of Bi2Se3 due to In incorporation will be reported. Synchrotron powder X-ray diffraction showed that a solid solution Bi2−xInxSe3 exists up to x = 0.8. Substituting Bi for In has a significant influence on the lattice parameters, volume and c/a ratio, as well as van der Waals gaps between two quintuple layers in the structure of ternary Bi2−xInxSe3. The crystal structure of the end composition of the solid solution, In0.8Bi1.2Se3, determined by single crystal X-ray diffraction will also be discussed in this presentation.

[1] Ghoumari H. et al. (1996). Materials Research Bulletin, 31, 177–187.
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