Electronic structure of Mn and Fe impurities in Bi-Sb-Te
BYUNGKI RYU, KYUNGHAN AHN, SANG MOCK LEE, KYU HYOU NG LEE, Samsung Advanced Institute of Technology — Bi$_2$Te$_3$-based thermoelectric materials are well known room temperature thermoelectric materials. Here we present a density-functional study of the electronic structure of Mn and Fe doped p-type Bi-Sb-Te (p-BST) to investigate the effect of metal impurities on the thermoelectronic properties. Our calculations show that, for both Mn and Fe, the substitutional impurity at the Bi/Sb-site is the most stable geometry. Mn is a single acceptor, whereas Fe is an isovalent defect. The metal $d$ bands are located within the host bands, not in the band gap. Due to the octahedral symmetry of the Bi/Sb-site, the metal $d$ bands of Mn and Fe are split into three $t_{2g}$ and two $e_{g}^*$ states in the high spin configuration. The electronic charge distribution analysis reveals that occupied $e_{g}^*$ states are well resonant with the host valence bands. As the $e_{g}^*$ states are located near the valence band maximum, Mn and Fe impurities are expected to enhance the p-type Seebeck coefficient of BST.

Byungki Ryu
Samsung Advanced Institute of Technology

Date submitted: 05 Nov 2012

Electronic form version 1.4