Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Theoretical study of defect properties in thermoelectric $(GeTe)_x(AgSbTe_2)_{1-x}$ HIKARI SHINYA, AKIRA MASAGO, TETSUYA FUKUSHIMA, HIROKI FUNASHIMA, HIROSHI KATAYAMA-YOSHIDA, Osaka Univ — We investigate the structural stability of a pseudo-binary alloy $(GeTe)_x(AgSbTe_2)_{1-x}$ called TAGS by the density functional theory. TAGS shows intermittent reductions of the thermal conductivity without change of the electric conductivity. However, the mechanism of the drastic change of the thermal conductivity has yet to be understood, and even the crystal structures are still under discussion. In this presentation, we will discuss these problems from a viewpoint of the structural stability. To clarify the stable structure, we estimate the formation energies of the point and the complex defects. As a result, a chain structure of Ag-Te-Sb in GeTe host crystal has a lower formation energy as compared to the homogeneous distribution. Moreover, the system becomes more stable by an assemblage of the chain structure. Furthermore, the calculated mixing energy shows that the system is favorable to the phase separation. In the phase separation, the grain boundary must play an important role in the large phonon scattering; therefore, it can lead to the thermal conductivity reduction. These calculations were done with Vienna ab initio Simulation Package and MACHIKANEYAMA2002 program package. [1] H. Shinya, et al., Jpn. J. Appl. Phys. 53, 111201(2014).

Hikari Shinya
Osaka Univ

Date submitted: 14 Nov 2014 Electronic form version 1.4