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First principles calculations of nanodots formation in high performance thermoelectrics AgPbmSbTem+2 HIROFUMI HAZAMA, Nagoya University, RYOJI ASAHI, Toyota Central R&D Labs., Inc., UICHIRO MIZUTANI, Nagoya University — Recently, $AgPb_mSbTe_{m+2}$ bulk thermoelectric material with a high figure of merit ZT over 2 was reported.[1] The excellent ZT mainly due to an enhancement of the Seebeck coefficient and a low thermal conductivity was resulted from simultaneous doping with Ag and Sb at the Pb site in PbTe. We have performed the first principles calculations to clarify effects of the Ag and Sb doping, in particular, on thermoelectric properties. The calculations have been done using the VASP-PAW method[2] within GGA. The lattice constants and atomic positions were fully optimized for different contents of doping; the obtained lattice constants were quite consistent with experiment. For $AgPb_{30}SbTe_{32}$system, we examined several configurations of Ag and Sb sites, giving the lowest total energy with a short distance between Ag and Sb. This results in preferable nanodots formation between Ag and Sb in $AgPb_mSbTe_{m+2}$, which were experimentally observed. The detailed calculations of the thermoelectric properties including Seebeck coefficients and thermal conductivities, emphasizing the effects of the nanodots formation, will be reported.
[1]K.F. Hsu et al., Science 303, 818 (2004). [2]G. Kresse et al., Comput. Mater. Sci. 6, 15 (1996).

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