Pressure-induced B1-to-B2 phase transition in $AgSbTe_2$: A first-principle study

E. Kim, R. Kumar, Y. Shen, A. Cornelius, and M. Nicol
Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154 (kimej@physics.unlv.edu)

We have performed density functional (DFT) calculations to investigate the pressure-induced B1-to-B2 phase transitions in functional gradient materials such as $AgSbTe_2$ and $AgSbSe_2$. B1-$AgSbTe_2$ phase is energetically stabler by 0.18 eV/atom than B2-$AgSbTe_2$ phase at ambient condition. The calculated lattice constant and bulk modulus of B1-$AgSbTe_2$ phase are 5.93 Å and 44.5 GPa, in excellent agreement with experimental results. Equation of state of B1- and B2-$AgSbTe_2$ phases indicates that B1-$AgSbTe_2$ phase is stable up to 16 GPa and B2- $AgSbTe_2$ phase becomes stable after 26 GPa, consistent with experiments. At the intermediate pressure between 16-26 GPa, our experimental data also implicate the existence of the intermediate phases on the way to the pressure-induced phase transition from B1 to B2 phase. Theoretical study of the possible intermediate states including amorphous phase is advanced, and pressure-induced structural phase transition of $AgSbTe_2$ is also under investigation.

This work was supported in part by the Department of Energy under Cooperative Agreement DE-FC08-01NV14049.