Abstract Submitted
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First principles study of thermoelectric properties of IV-VI semiconductor superlattices[1] P.D. BORGES, Universidade Federal de Vicosa, Brazil, J.E. PETERSEN, L. SCOLFARO, Texas State University, USA, H.W. LEITE ALVES, Universidade Federal de Sao Joao del Rei, Brazil, T.H. MYERS, Texas State University, USA — Thermoelectric materials (TE) have attracted great attention due to their ability to convert heat directly into electricity. However, to be commercially competitive with existing technology, TE devices must have a higher value of figure of merit ZT. It has been proposed to improve ZT by using multilayered systems or superlattices (SLs) resulting in 1D or 2D carrier confinement, reduction of the phonon thermal conductivity, and introduction of anisotropy effects. Here we study the TE properties of IV-VI derived semiconductor SLs. By using the Boltzmann transport theory, within the constant scattering time approximation, in conjunction with first principles calculations, we study the Seebeck coefficient (S) and ZT of PbTe/SnTe SLs. The calculated S shows good agreement with recent experimental data. An anisotropic behavior is observed for low carrier concentrations less than 10ˆ18cmˆ-3. For T = 900 K, a large value of ZT parallel to the SL axis equal to 2.6 is predicted for n=1.2x10ˆ18cmˆ-3, whereas ZT perpendicular to the SL axis peaks at the value 1.4 for n=5.5x10ˆ17 cmˆ-3. Both electrical conductivity enhancement and reduction of thermal conductivity are analyzed, and a comparison with other multilayered systems such as planar-doped PbTe is done.

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