ABSTRACT

The ab-initio calculations were performed using density functional theory (DFT) as implemented in the Quantum ESPRESSO (QE) code. Lattice parameter mismatch was minimal (2.5 % - 3 %) in TiNiSn/TiNi2Sn, ZrNiSn/ZrNi2Sn, and HfNiSn/HfNi2Sn compounds. Half-Heusler compounds had shorter bond lengths and smaller bulk moduli than their full-Heusler counterparts. Directional dependencies of the Young's and shear moduli were investigated using elastic constants. TiNiGe, HfNiSn, and ZrNiSn had a greater universal anisotropy index among the half-Heusler compounds. Half-Heusler, TiNi2Sn, TiNi2Si, ZrNi2Sn, and HfNi2Sn compounds are reported to be dynamically stable. The electronic structure computations show that TiNiSn, ZrNiSn, and HfNiSn compounds have the least indirect energy gaps of 0.4508 eV, 0.5019 eV, and 0.3847 eV respectively. TiNiSn, ZrNiSn, and HfNiSn compounds are good candidates for minimizing the thermal conductivity of thermoelectric devices. TiNi2Sn, ZrNi2Sn, and HfNi2Sn are good candidates as possible contact electrodes for TiNiSn, ZrNiSn, and HfNiSn.