Theoretical investigations of NiTiSn and CoVSn compounds

Abstract

The structural, elastic and electronic properties of NiTiSn and CoVSn half-Heusler compounds have been calculated using the full-potential linear muffin-tin orbital (FP-LMTO) method. The computed equilibrium lattice constants are in excellent agreement with the available experimental and theoretical data. The elastic constants C_{ij} are calculated using the total energy variation with strain technique. The polycrystalline elastic moduli (namely: the shear modulus, Young's modulus, Poisson's ratio, Lamé's coefficients, sound velocities and the Debye temperature) were derived from the obtained single-crystal elastic constants. The ductility mechanism for the studied compounds is discussed via the elastic constants C_{ij} and their related parameters. The electronic band structure calculations show that the conduction band minimum (CBM) is located at the X point for both compounds, whereas the valence band maximum (VBM) is located at the point for NiTiSn and at the L point for CoVSn, resulting in indirect energy band gaps of 0.46 and 0.75 eV for NiTiSn and CoVSn, respectively. The pressure and volume dependences of the energy band gaps have been calculated.