First-principle calculations to investigate the elastic and thermodynamic properties of $RBRh_3$ (R =Sc, y and La) perovskite compounds

Abstract

We have performed first-principle calculations using the full-potential linear augmented plane wave (FP-LAPW) method within density functional theory (DFT) to investigate the structural, elastic and thermodynamic properties of the cubic perovskite $RBRh_3$ (R=Sc, Y and La) compounds. The exchange-correlation potential is treated within the generalized gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE). Single-crystal elastic constants are calculated using the total energy variation versus strain technique, then the shear modulus, Young's modulus, Poisson's ratio and anisotropic factor are derived for polycrystalline $RBRh_3$ using the Voigt-Reuss-Hill approximations. Analysis of the calculated elastic constants and B/G ratios shows that these compounds are mechanically stable and ductile in nature. Using the quasi-harmonic Debye model, the effect of pressure P and temperature T on the lattice parameter a_0, bulk modulus B_0, thermal expansion coefficient , Debye temperature and the heat capacity C_v for these compounds are investigated for the first time. The computed structural and elastic constants are in good agreement with the available experimental and theoretical data.