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 $\alpha$, 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.