The effect of chalcogen atom on the structural, elastic, and high-pressure properties of XY compounds (X=La, Ce, Eu, and Y=S, Se, and Te): An ab initio study

Abstract

The B1 (NaCl) and B2 (CsCl) structure of rare-earth monochalcogenides XY (X=La, Ce, Eu, and Y=S, Se, and Te) were investigated with the full-potential linearized-augmented plane wave (FP-LAPW) scheme in the frame of the generalized gradient approximation (GGA). The optimized lattice parameters, independent elastic constants (C_{11}, C_{12}, and C_{44}) at zero and high pressure, bulk modulus B, and its pressure derivative and the shear modulus G were evaluated. Further, the numerical estimates of a set of elastic parameters [Young's modulus E, Poisson's ratio (ν), Lame's coefficients (μ, λ)] of the polycrystalline XY (X=La, Ce, Eu, and Y=S, Se, and Te) compounds (in the framework of the Voigt-Reuss-Hill approximation) were performed. The pressures at which these compounds undergo structural phase transition from B1 (NaCl) to B2 (CsCl) phases were calculated. For rare-earth monochalcogenides XY, the Debye temperature is also estimated from the average sound velocity.