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External temperature and pressure effects on thermodynamic properties and mechanical stability of yttrium chalcogenides YX(X=S, Se and Te)

Abstract

The full potential linearized augmented plane wave method within the framework of density functional theory is employed to investigate the structural, thermodynamic and elastic properties of the yttriumchalcogenides (YX: X=S, Se, and Te) in their low-pressure phase (Fm3m) and high-pressure phase (Pm3m). The exchange-correlation potential is treated with the generalized gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE). Temperature dependence of the volume and both adiabatic and isothermal bulk moduli is predicted for a temperature range from 0 to 1200 K for the both phases of the here in considered materials. Furthermore, we have analyzed the thermodynamic properties such as the heat capacities, CV and CP, thermal expansion, a, and Debye temperature, ΦDi under variablepressure and temperature. We have calculated the isothermal elastic constants QjT of the YXmonochalcogenides in both NaCl-B1 and CsCl-B2 phases at zero pressure and a temperature range 0-1200 K. The results show that rare earth yttrium monochalcogenides are mechanically stable at hightemperature. The elastic anisotropy of all studied materials in the two phases has been studied using three different methods.

Keywords

Elastic constants; FP-LAPW; GGA; Structural properties; Thermodynamic properties; Yttrium monodialcogenides