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Elastic and thermodynamic properties of ZnSc2S4 and CdSc2S4 compounds under pressure and temperature effects

Abstract

Results of ab initio calculations of the lattice parameter, elastic constants and some thermodynamic parameters in a wide range of pressures and temperatures are reported for the ZnSc2S4 and CdSc 2S4cubic spinels. The calculated equilibrium lattice parameters are compared with available experimental data. Elastic constants and some related properties for single-crystal and polycrystalline have been calculated at zero pressure and zero temperature using the analysis of changes in calculated stresses resulting from changes in strain. Evolution of the elastic constant with pressure and temperature is predicted. From the ab initio calculated total energy versus volume and using the quasi-harmonic Debye model, in which the phononic effects are taken into account, the evolution of some thermodynamic parameters with temperature and pressure is computed. This is the first quantitative theoretical prediction of the reported properties and it still awaits experimental confirmation.

Keywords

Spinel sulfides; Ab initio calculations; Elastic constants; Pressure effect; Thermal effect; Thermodynamic properties