

The influence of pressure on half-metallicity, magnetism and thermomechanical properties of Fe-based Heusler alloys

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Abstract

The half-metallicity of Heusler alloy is quite sensitive to high pressure and disorder. Therefore, we systematically studied the half-metallic nature, magnetism and thermomechanical properties of FeCrTe and FeCrSe Heusler alloys under high pressure using ab initio calculations based on density functional theory (DFT). The ground state lattice constants for FeCrTe and FeCrSe alloys are 5.93 and 5.57 Å, consistent with available theoretical results. The formation energy, cohesive energy and elastic constant confirmed the thermodynamically and mechanical stability of both compounds. The FeCrTe and FeCrSe alloys showed half-metallic character with the band gap of 0.68 and 0.58 eV at 0 Gpa pressure respectively and magnetic moments of 2.01 μ_B for both alloys using GGA approximation. The elastic properties have been scrutinized and found that FeCrTe is ductile and FeCrSe is brittle at 0 Gpa pressure. Under pressure, FeCrSe turn into brittle above 10 Gpa pressure. Moreover, the average sound velocity V_m , Debye temperature D and heat capacity CV were predicted under pressure. These outcomes would advantage in integrating Fe-based half-Heusler alloys in spintronic devices.

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