Density functional investigation of electronic structure, magnetic and structural properties of several Heusler alloys

Wenxu Zhang, Klaus Koepernik, Ulrike Nitzsche, Manuel Richter
Leibniz-Institute for Solid State and Materials Research, IFW Dresden, P.O. Box 270016,D-01171 Dresden,Germany

The lattice parameters,electronic structure, and magnetic moments of several Heusler alloys with cubic and tetragonal structures are studied by scalar relativistic full-potential local-orbital minimum basis band structure calculations. The influence of hydrostatic pressure on these properties is investigated. The calculation reveals that the cubic structure of one of the compounds is unstable at zero temperature, and the tetragonal structure has a lower energy. The predicted martensitic phase transformation from the higher temperature cubic phase to the lower temperature tetragonal phases can be understood as a band Jahn-Teller effect. The tetragonal distortions can lower the energy by splitting a peak of the density of states which is situated at the Fermi level in the cubic structure.

9.7 cm

13.4 cm

Subject category :
7. Computations of Electronic Structures

Presentation mode :
poster

Corresponding author :
Wenxu Zhang

Address for correspondence :
Leibniz-Institute for Solid State and Materials Research, IFW Dresden, P.O. Box 270016,D-01171 Dresden,Germany

Email address :
wenxu.zhang@ifw-dresden.de