Modeling thermal expansion of Ni_2MnGe

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9.7 cm

Thermal expansion is important property in numerous applications.
In ferromagnet/semiconductor heterostructures, in which the some Heusler alloys have been recently used, stresses may be generated at the interfaces due to thermal expansion mismatch.
The present study of Ni_2MnGe is focused on describing the thermal properties of the alloy in a framework of first-principles electronic structure calculations coupled with a Debye treatment of the vibrating lattice. The presented Ni_2MnGe Heusler alloy has the cubic $L2_1$ structure. The electronic structure of Ni_2MnGe has been studied using the full-potential nonorthogonal local-orbital minimum basis method (FPLO). The total energy of the system is found in the full-relativistic calculations based on the first-principles density of states theory (DFT) with the exchange-correlation potential of the Perdew-Wang parametrisation. The theoretical lattice parameter obtained from the dependence of the total energy on the lattice parameter is in agreement with experimental one. In order to make the prediction of the thermodynamic properties of Ni_2MnGe the Debye-Grüneisen model was chosen to account for the vibrational contribution and calculate the coefficient of linear thermal expansion. Two approximations for Grüneisen parameter γ, i.e. Slater's and Dugdale and MacDonald's expressions were assumed.

13.4 cm

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