Ab initio Calculations of Phase Transformations in $Ni_{50}Mn_{50-x}Sn_x$ Heusler Alloys

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9.7 cm

Ferromagnetic Shape Memory Alloys (FSMA) are characterized by martensitic transformation in a ferromagnetic state. The Ni-Mn-X (X = In, Sn, Sb) systems with an excess of Mn atoms are off-stoichiometric Heusler alloys which exhibit shape memory effect. The present study is focused on $Ni_{50}Mn_{50-x}Sn_x$ systems whith $L2_1$ structure in the high temperature austenite phase and with a lower symetry martensite phase (orthorhombic or tetragonal) at low temperatures. We present results of band structure calculations based on Full-Potential SPR-KKR-CPA [1-3]. The total energy of $L2_1$ structure as a function of volume and c/a ratio is presented. The c/a ratio calculations were done for constant, optimal unit cell volume. The total magnetic moment and its contributions as a function of c/a are also presented. For the sake of comparison the total energy as a function of c/a ratio calculated with Atomic Sphere Approximation (ASA) is presented.

[1] *The Munich SPR-KKR package, version 5.4*, H. Ebert et al.
[2] http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR
[3] H. Ebert, *Fully relativistic band structure calculations for magnetic solids Formalism and Application, in Electronic Structure and Physical Properties of Solids*, editor: H. Dreyssé, Lecture Notes in Physics, vol. 535, p. 191, Springer Berlin

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