Magnetic and magnetocaloric properties of Pd_2MnZ (*Z*=Ga, As, Sb) Heusler alloys: theoretical study

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Heusler alloys exhibit a number of remarkable properties such as shape memory effect, effects of superplasticity and superelasticity, giant magnetocaloric effect, giant magnetoresistance and magnetostrain, etc. The above properties are associated with martensitic transformations [1-4]. Among Heusler alloys, Pd-based compounds are underexplored. However, they were chosen to search for new compositions in technology of magnetic cooling because magnetic and phase transitions are possible in these alloys, and as a consequence, thermal effects.

In this work, we present a theoretical study of magnetic and magnetocaloric properties of Pd_2MnZ (*Z*=Ga, As, Sb) Heusler alloys with the help of the microscopical approach consisting of ab initio zero-temperature calculations combined with Monte Carlo finite-temperature simulations. At the first stage, we carried out the ab initio supercell calculations of ground state properties (lattice parameters, magnetic order, magnetic moments, exchange coupling constants for austenite and martensite). At the second stage, Monte Carlo simulations of temperature dependences of magnetic and magnetocaloric properties for alloys studied by means of Potts-Blume-Emery-Griffiths model were performed [5]. For Pd_2MnSb coupled magnetostructural transition from ferromagnetic martensitic state to paramagnetic austenitic state is predicted. In whole, the theoretical results are in a good agreement with available experimental data.

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