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EFFECT OF LATTICE COMPRESSION ON MAGNETIC PROPERTIES OF THE MnNiGe-BASED MAGNETOCALORIC ALLOYS. II. *Ab initio* STUDY

Within the *ab initio* calculations of the spin-polarized electronic structure of MnNiGe and related compounds, the reasons and the conditions for transition from a spiral magnetic structure stable in the ground state to the ferromagnetic ordering are investigated. Such transitions are observed experimentally at certain kinds of cationic and anionic substitution in MnNiGe, and under pressure. It is shown that simple contraction of the MnNiGe lattice to the level of MnCoGe is sufficient for the emergence and stabilization of the ferromagnetic state. In the case of MnCoGe, the increase of the lattice parameters to the MnNiGe level produces inverse action, that is, the observed change in the type of magnetic ordering determined mainly by changing the parameters of the crystal lattice.

The estimations of the value of pair interatomic exchange interactions between magnetic atoms in orthorhombic MnNiGe were done. Short-range nature of these interactions strongly affected by the type of magnetic ordering in the crystal is found, which indicates their non-Heisenberg nature and should be considered in the correct modeling of magnetic behavior of these materials. Attainability of the half-metallic ferromagnetic state in orthorhombic MnNiGe is detected which means 100% of electron polarization that can be used in spintronics.

Keywords: electronic structure, semi-metals, ferromagnets, double helix, interatomic exchange interactions, magnetocaloric effect.

Fig. 1. Crystal lattice of the MnNiGe orthorhombic phase (spatial group *Pnma*, crystal structure of the TiNiSi type)

Fig. 2. Spin-polarized electron structure of certain semi-Heisler alloys with orthorhombic lattice of the TiNiSi type in hypothetic (for MnNiGe and MnCoSi) and real (for MnCoGe) FM-state. Calculations were preformed for experimental low-temperature values of lattice parameters: *а* – MnCoGe (4.2 K), *б* – MnCoSi (4.2 K), *в* – MnNiGe (80 K), *г* – MnNiGe (4.2 K)

Fig. 3. Spin-polarized density of the electron states of MnNiGe near Fermi level at varied wave vector Q of the spiral magnetic structure. Lattice parameters correspond to the experimental values at 4.2 K: — – $Q = 0$, --- – $Q = 0.5\pi$/a, ··· – $Q = \pi/a$

Fig. 4. Wave vector dependence of the energy of spiral magnetic structure of *a*-type for MnNiGe (■, □) and MnCoGe (▲, △). Dark symbols correspond to the experimental lattice parameters of MnNiGe at $T = 4.2$ K ($a = 6.0435$ Å, $b = 3.7165$ Å, $c = 7.083$ Å); blank symbols mark MnCoGe at $T = 4.2$ K ($a = 5.894$ Å, $b = 3.798$ Å, $c = 7.035$ Å). The arrows indicate experimental values of Q observed in MnNiGe at 12 K ($Q = 0.185 \cdot 2\pi/a$) and 293 K ($Q = 0.228 \cdot 2\pi/a$)

Fig. 5. Interatomic distance dependence of pair exchange interactions between magnetoactive atoms in MnNiGe for hypothetic FM-state (dark symbols) and AF-state (blank symbols). The interacting pairs: ■, □ – Mn_1–Mn_1; ●, ○ – Mn_1–Mn_2; ▲, △ – Mn_1–Mn_3. Numbering of atoms corresponds to that of Fig. 1