

**AB INITIO STUDY OF ELECTRONIC, MAGNETIC
STRUCTURE AND STRUCTURAL PHASE TRANSITION
OF $(\text{Fe}_{1-x}\text{Mn}_x)_2\text{P}_{1-y}\text{Ge}_y$ ALLOYS**

J. Deniszczyk^a, A. Woźniakowski^a, R. Kolano^b, A. Kolano-Burian^b

^aInstitute of Materials Science, University of Silesia, 40-007 Katowice, Poland

^bInstitute of Non-Ferrous Metals, 44-100 Gliwice, Poland

Transition-metal and rare-earth based multicomponent intermetallic alloys are subject of intensive investigations due to their potential applications for magnetocaloric devices. In the $(\text{Fe}_{1-x}\text{Mn}_x)_2\text{P}_{1-y}\text{Ge}_y$ alloys it was found that the magnetic phase transition is accompanying by the first order isostructural phase transition, modifying the lattice parameters and atomic positions. The coexistence of the two phase transition results in a high magnitude of magnetic entropy change induced by magnetic field. This feature predestined the alloy for magnetocaloric applications.

In this paper we present the results of *ab initio* electronic and magnetic structure calculations performed for $(\text{Fe}_{0.5}\text{Mn}_{0.5})_2\text{P}_{0.67}\text{Ge}_{0.33}$, $(\text{Fe}_{0.58}\text{Mn}_{0.42})_2\text{P}_{0.83}\text{Ge}_{0.17}$ and $(\text{Fe}_{0.5}\text{Mn}_{0.5})_2\text{P}$ structures. The electronic structure calculations were carried out with the use of the DFT based FP-LAPW method implemented in the WIEN2k code. The GGA-LSDA form of exchange-correlation potential was applied. To elucidate the nature of isostructural phase transition the Fixed Spin Moment approach was utilised. Total energy analysis confirmed the occurrence of isostructural phase transition for the value of magnetization which coincides with the observed one. Moreover calculations reveal the change of magnetic order from ferromagnetic to ferrimagnetic type accompanying the structural phase transition.

13.4 cm

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Corresponding author :

Józef Deniszczyk

Address for correspondence :

Institute of Materials Science, University of Silesia
Bankowa 12, 40-007 Katowice, POLAND

Email address :

jozef.deniszczyk@us.edu.pl

9.7 cm