ATOMIC DISORDER IN SOME HEUSLER ALLOYS

A. Jezierski[a], **P. Kowalewski**[a], **A. Ślebarski**[b], **A. Wrona**[b]

[a]Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

[b]Institute of Physics, University of Silesia, Katowice, Poland

We report the influence of the local atomic disorder on the magnetic properties and electronic structure of $Ni_2(Mn_xTi_{1-x})Sn$, $Fe_{2-x}Ni_xTiSn$, $Fe_{2-x}Co_xTiSn$ and Fe_xTiSn Heusler type alloys. The electronic and magnetic properties are calculated by the spin–polarised TB LMTO method in the atomic sphere approximation (ASA) within the local–spin density approximation (LSDA). The substitution of Fe atoms onto titanium or tin positions leads to an increase of the magnetic moment. Fe_2TiSn is a nonmagnetic material whereas for the disorder alloy the magnetic ground state is obtained, in agreement with observation. The theoretical lattice parameter estimated from the minimum of the total energy for $x \geq 1.5$ was very similar to that obtained experimentally by X–ray diffraction on the Fe_xTiSn samples. In $Ni_2(Mn_xTi_{1-x})Sn$ alloy we found the critical concentration x for which the system was magnetic.

9.7 cm

13.4 cm

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Corresponding author :

A. Jezierski

Address for correspondence :

Institute of Molecular Physics, Polish Academy of Sciences,
ul. M. Smoluchowskiego 17,
60–179 Poznań, Poland

Email address :

jeziersk@ifmpan.poznan.pl