Сплавы с эффектом памяти формы: свойства, технологии, перспективы

## AB INITIO INVESTIGATION OF STRUCTURE AND MAGNETIC PROPERTIES OF Ni<sub>2</sub>MnGa AND Co<sub>2</sub>MnGa COMPOUNDS Breczko T.<sup>1</sup>, Dłużewski P.<sup>2</sup>, Tamuliene J.<sup>2</sup>

<sup>1</sup>University of Bialystok, Sosnowa str. 64, 15-887 Bialystok, Poland <sup>2</sup> Institute of Fundamental Technological Research (IPPT PAN), Pawińskiego 5 B, 02-106

Warszawa

<sup>3</sup>Vilnius University, Institute of Theoretical Physics and Astronomy, A. Gostauto 12, LT -01108 Vilnius, Lithuania

tbreczko@uwb.edu.pl

Half-metallic ferromagnets have been produced and studied as ideal candidates for the magnetoelectronic and spintronic devices. Among many half-metallic ferromagnets special attention has been drown on Heusler alloys such as Ni<sub>2</sub>MnGa and Co<sub>2</sub>MnGa that show high Curie temperature and high spin polarization [1]. Several studies by means of X-ray and neutron diffraction measurements indicate that the alloys present L2<sub>1</sub> structures with mainly ferromagnetic ordering [2]. However, R. J. Kim and et al. found a well-ordered crystalline state, a disordered state and crystalline state with an intermediate order and exhibited influence of the structural order on the physical properties of the Co<sub>2</sub>MnGa films [3]. The similar phenomena for Ni<sub>2</sub>MnGa are described in work [4]. The results of our recent theoretical investigations of these compounds consist of eight lattices prove the presence of the disordered and ordered structures in the above compounds. The results obtained indicate Co<sub>2</sub>MnGa and Ni<sub>2</sub>MnGa as compounds possessed a cubic lattice. However, the 8 cubic lattices form the ordered structure in Co<sub>2</sub>MnGa and disordered in Ni<sub>2</sub>MnGa. 'Disordered' means that the cubic lattices of the Ni compound are shifted in respect each other (Fig.1)

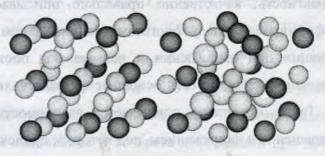


Figure 1. View of the  $Co_2MnGa$  structure investigated on the left and that of  $Ni_2MnGa$  on the right. Co or Ni is marked by light grey cycle, Ga- grey Mn- black

## Сплавы с эффектом памяти формы: свойства, технологии, перспективы

The analysis of the charge distribution, bond orders and lengths indicates different electronic structure of the compounds although their magnetic properties are similar [5]. Hence the questions arisen: do the obtained structures take place in the periodic structure, i.e. the structures obtained is translated; do the disorder obtained in experiments is related with cubic cell shift as it is found in the case of Ni compounds; are the charge and spin distributions of the above structures took place in periodic structure, too; are differences of the magnetic properties of these compounds investigated obtained in the periodic structures.

To answer the above questions we perform investigation of the periodic structure of the Co<sub>2</sub>MnGa and Ni<sub>2</sub>MnGa compound by using state-of-the-art computational ab-initio methods.

2. Ayuela, J. Enkovaara, K. Ullakko, R. M. Nieminen, J.Phys.: Condens. Matter 11 (1999).

- 4. Alexey T. Zayak, Ph.D. thesis 'A first-principles investigation of the magnetic, structural and dynamical properties of Ni<sub>2</sub>MnGa" (2003).
- 5. T. Breczko, J. Tamuliene, Investigation of electronic structure of heusler alloys: cubic and tetragonal cells, accepted for publication in Materials physics and mechanics. St. Petersburg : Institute of Problems of Mechanical Engineering (2013)

явач дя неолнородных напряженных состояный, которые могли бы слидерстотновае

Урасные залиси для СТФ задовска в высокой внейски необности проблем и нестоянойски волска работ Чекату зокала таких проблем и Консерсания улизикание системы исланование уданналия. Для решение таких проблем и Консерса - для неять власта на пользонаущего работ найор, парасстрикание израние произоры, ото рекото нанкит от выбора скены инфортизаростров слащности. Поректров, мар васто нанкит от выбора скены инфортизация и таких расский улих премытра, общество васто нанкит от выбора скены инфортизация и тактений этих произоры, общество васто нанкит от выбора скены инфортизации и таких расский этих поректров общество из таких на расского на скены инфортизации и таких поректров общество и таких на расского на скены инфортизации и таких поректров общество и таких на расского на скены инфортизации и таких на расского на расского

(т. В.), полорія для СОФ, Разнанскої на полощити полоції, корання станції и полоції, країнсь стана полощих станах станцих станцих станцих, полощих станах станах станцих станцих, станцих, станцих, станцих, станцих, полощих полощих полощих станах станах станцих, полощих полощ

<sup>1.</sup> S. Fujii, S. Sugimura, S. Ishida, S. Asano, J. Phys: Condens. Matter 2, 8583 (1990)

<sup>3.</sup> R. J. Kim Y. J. Yoo, K. K. Yu, T. U. Nahm, Y.P. Lee, Y.V. Kudyavtsev, V. A. Oksenenko, J. Y. Rhee, K.W. Kim, Joural of the Korean Physical Society, 49, 3 (2006).