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Comparative Study of Compressibility of Ni_2MnX (X=In, Sn, Sb) Heusler Alloys

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The present study is focused on the compressibility of Ni_2MnX (X = In, Sn, Sb) Heusler alloys, which were investigated from the first principles. The study of the pressure effect on the magnetic properties of Ni_2MnX (X = In, Sn, Sb) predicted the decrease in the total magnetic moment from ambient pressure to pressure above 20 GPa.

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1. Introduction

An increasing interest in the Heusler alloys has been motivated by the search of ferromagnetic materials suitable for application in spintronic devices [1] or for magnetic actuator [2]. An understanding of the mechanical behaviour of some materials is also important for their applications. *Ab initio* calculations provide a microscopic framework to study the cohesion and deformation behaviour of these systems. Effect of hydrostatic pressure on the Curie temperature (T_C) for Ni_2MnX (X = Al, Ga, In, Sn, Sb) has been experimentally studied in [3]. The change of magnetisation of $Ni_{2-x}Mn_{1-x}Ga$ experimentally studied on pressure [4] is consistent with features of electron band structure of the alloy. The isothermal compressibility and the Mössbauer high-pressure experiments of Ni_2MnSn have been performed by Gavriliuk et. [5]. Moreover, increase in the experimental value of T_C with pressure in Ni_2MnSn [5] is well confirmed by *ab initio* calculations [6]. The present *ab initio* studies are addressed to cohesive properties of Ni_2MnX (X = In, Sn, Sb) (equilibrium lattice constant, cohesive energy), the mechanical properties (bulk modulus, its derivative) and to pressure behaviour of magnetic moments.

2. Method of calculation

The ground state calculations were performed using the full-relativistic calculations in the full-potential nonorthogonal local-orbital minimum basis (FPLO)

scheme [7, 8] with exchange-correlation potential in the form from [9]. The studied alloys have cubic $L2_1$ structure. The lattice contains four interpenetrating fcc sublattices at positions (0,0,0) for Mn,$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, $(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$ for Ni and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ for X (X = In, Sn, Sb). Ni 4s, 4*p*, 3*d* states, Mn 4*s*, 4*p*, 3*d* states, In, Sn, Sb 5*s*, 5*p*, 4*d* states, were chosen as a minimum-basis set for the valence states. The Brillouin zone integrations were performed using the tetrahedron method and 732 k-points used in its irreducible part.

3. Results and discussion

The performed calculations clearly favour the ferromagnetic ground state for Ni_2MnX (X = In, Sn, Sb). We have optimized the lattice parameters for studied series in $L2_1$ structure and calculated their cohesive energies (E_{coh}). E_{coh} is an energy required to separate components of a compound into neutral free atoms. E_{coh} of the compounds is calculated as the total energy difference between the elemental components and the compound at equilibrium lattice constant. The calculated values of the E_{coh} of the studied alloys are given together with the equilibrium lattice parameters in Table. We pointed out that the determination

TABLE

The theoretical equilibrium lattice parameters (a) in [Å], cohesive energies (E_{coh}) [Ry/f.u.], bulk modulus (B) in [GPa], its derivatives (B') and magnetic moments (m) in [μ_B] of Ni_2MnX (X = In, Sb, Sn)

x	a	E_{coh}	B [GPa]	B'	m
Ni_2MnIn	5.96	2.7452	168.5	4.2	4.05
Ni_2MnSn	5.92	2.8233	168.5	2.9	3.86
Ni_2MnSb	6.0	2.8317	168.3	6.0	3.87

of lattice parameter from minimum of the total energy for Ni_2MnX (X = In, Sn, Sb) yields results that are systematically somewhat smaller than the experimental values [10]. *Ab initio* calculations are strictly valid at absolute zero (T = 0 K) which should explain some observed differences between the theoretical results and experimental values of lattice parameter as well as magnetic moments [3, 10]. The bulk modulus expresses the material resistance to hydrostatic pressure. The total energy dependences on the cell volume for studied Ni_2MnX are fitted by the Murnaghan equation of state (EOS) [11] to obtain bulk modulus (B) and its pressure derivative (B'). Its values are summarised in Table. The obtained values of B for Ni_2MnSn and Ni_2MnIn are higher than achieved in other *ab initio* studies [2, 12]. This may reflect the fact that different first principles methods were used as well as fact that presented results were obtained on the assumption of spin–orbit

interaction. The pressure–volume relation for studied systems was calculated as the negative volume derivative of the total energy. The isothermal (at $T = 0$ K) pressure–volume relationship is shown in Fig. 1. Figure 2 illustrates the change of

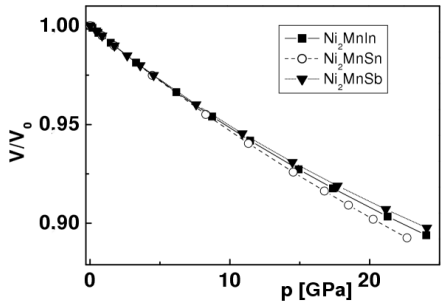

Fig. 1. The p–V relation for Ni_2MnX (X = In, Sn, Sb).

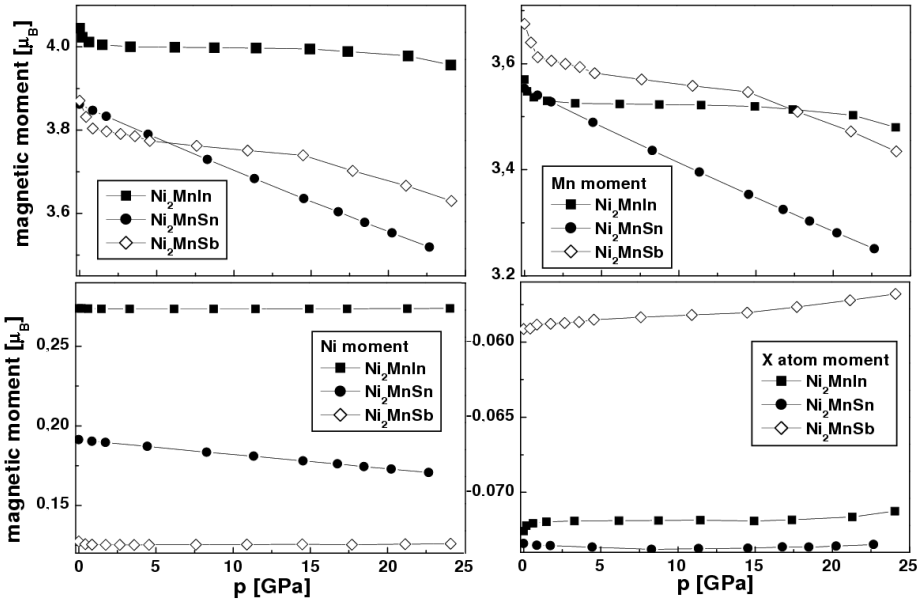

Fig. 2. The pressure dependence of the total and local magnetic moments in Ni_2MnX (X = In, Sn, Sb).

the total and the local spin magnetic moments with pressure. The linear decrease in the total magnetic moment with pressure for Ni_2MnSn is in good agreement with previous calculation [6]. For Ni_2MnIn and Ni_2MnSb the response of the total moment to pressure is initially nonlinear and is connected with behaviour of Mn moment under pressure. The pressure leads to a slight shift of $3d$ Mn peaks to

lower energy and to decrease in magnitude of these peaks. In the low pressure region the magnitude of $3d$ Mn bonding peaks decreases faster for Ni_2MnSb than for Ni_2MnIn. In Ni_2MnSb it causes a decrease in majority density of states of Mn as well as very sharp decrease in Mn moment at low pressure below 2 GPa. For these both alloys Ni moment has practically the same value (0.274 μ_B for Ni_2MnIn and 0.127 μ_B for Ni_2MnSb) in whole studied pressure region. For Ni_2MnSn Ni moment changes from 0.19 μ_B at ambient pressure to 0.17 μ_B at 20 GPa. Although the value of Ni moment for Ni_2MnSn is less than in [6] the pressure behaviour of the moment is the same. The induced moment on X atoms is opposite to the Mn and Ni moment. Its value slightly increases with pressure for studied Ni_2MnX.

4. Conclusions

Using the FPLO *ab initio* method we have determined bulk modulus, its derivatives, cohesive energies, and volume–pressure relation for series Ni_2MnX. The obtained bulk modulus of Ni_2MnIn and Ni_2MnSn is larger than in previous calculations. It may follow from the fact that spin–orbit interaction was included in total energy calculations. A good agreement of linear behaviour of the total magnetic moment of Ni_2MnSn is found with the available *ab initio* results. For Ni_2MnIn and Ni_2MnSb the presented study predicts nonlinear pressure–magnetization relation for pressure from 0 GPa to 15 GPa.

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