Prospects for controlling the magnetic properties of Ni_2MnAl upon substitution with excess Mn in Ni site. DFT studies

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Despite extensive studies of the shape-memory Ni_2MnGa alloy, numerous other Ni_2-based Heusler alloys continue to attract significant interest owing to their multifunctional properties. In Heusler compounds, the magnetic shape-memory effect generally originates from a thermoelastic martensitic transition from the cubic $L2_1$ structure to a phase with lower symmetry, most commonly a tetragonal distorted phase. Martensitic transitions have been reported in the literature [1] for ferromagnetic $Ni_2Mn_{1+x}Z_{1-x}$ alloys with an excess of Mn occupying the Z sublattice (where Z = *sp* elements).

The Ni_2MnAl compound has been proposed as a promising candidate for applications requiring precise property tuning via atomic substitution. Therefore, using a Ni-to-Mn substitution strategy, first-principles calculations of the magnetic properties of $Ni_{2-x}Mn_{1+x}Al$ are presented in this work. Although one component of the magnetic shape-memory effect observed experimentally involves a structural transformation from the cubic phase to a lower-symmetry structure upon cooling, the present theoretical study is restricted to the high-temperature cubic phase. The results confirm the mechanical stability of the selected cell configurations upon Ni–Mn substitution. The calculated elastic constants provide a basis for further investigation of the transition from the cubic phase to a tetragonally distorted structure. Futermore, based on the obtained results, the influence of hydrostatic pressure on the linear behavior of local magnetic moments on Mn atoms in two crystallographically ineqiuvalent sublattices is discussed.

The calculations were performed using the Vienna ab initio Simulation Package (VASP) [2] within the framework of density functional theory (DFT). The electron–ion core interaction was described using the projector augmented wave (PAW) method [3]. Exchange and correlation effects were treated using the Perdew–Burke–Ernzerhof (PBE) [4] functional within the generalized gradient approximation (GGA).

References:

[1] Y. Sutou, Y. Imano, N. Koeda, I. Omori, R. Kainuma, K. Ishida, K. Oikawa, Appl. Phys. Lett. 85, (2004) 4358.

[2] G. Kresse, J. Hafner, Phys. Rev. B 47 (1993) 558, G. Kresse, J. Hafner, Phys. Rev. B 49 (1994) 14251, G. Kresse, J. Furthmüller, Phys. Rev. B 54 (1996) 11169,.

[3] P.E. Blöchl, Phys. Rev. B: Condens. Matter Mater. Phys. 50, (1994) 17953.

[4] J.P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 77 (1996) 3865.