AB INITIO ANALYSIS OF ISOTROPIC STRENGTH AND ELASTICITY OF NICKEL ALUMINIDE COMPOUNDS

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In the past two decades, an extensive experimental and theoretical attention was paid to intermetallic compounds and ordered alloys. In particular, nickel aluminide (Ni_xAl_y) was studied by many authors, e.g. [1,2]. Unique mechanical properties of Ni_xAl_y, attractive for structural applications, were the main reason for this interest.

In this paper, the influence of chemical composition on the elastic response of Ni_xAl_y under isotropic deformation is theoretically studied in terms of the crystal energetics. A pure Ni, Ni_3Al, $NiAl$, $NiAl_3$ and a pure Al were selected as representative Ni_xAl_y compounds. Various crystal structures (phases) are considered for each compound and the ground state structure is found as that of the lowest energy.

Bulk elastic moduli B and the equilibrium lattice parameters a_0 are computed and crystal stability is analyzed at the inflexion point of the dependence of the total energy on the volume. The energy can be expressed as a function of the Lagrangian deformation tensor as

$$E = E_0 + V\sum_{ij}\sigma_{ij}\eta_{ij} + \frac{1}{2}V\sum_{ij}\sum_{kl}C_{ijkl}\eta_{ij}\eta_{kl} + O(\eta^3),$$

where V is the crystal volume, σ_{ij} is component of a stress tensor, η_{ij} are components of the strain tensor and C_{ijkl} are the elastic moduli. Using this energy expansion, the elastic moduli can be calculated as

$$C_{ijkl} = \frac{1}{V}\frac{\partial^2 E}{\partial\eta_{ij}\partial\eta_{kl}}.$$

Under the isotropic deformation, the simple relation $\eta_{ij} = \eta\,\delta_{ij}$ for strain tensor components leads to

$$B = \frac{1}{3}(C_{11} + 2C_{12}) = \frac{1}{9V}\frac{\partial^2 E}{\partial\eta^2}.$$

The total energy is computed by means of ab-initio approach. Namely, the code based on the linear muffin tin orbital method in the frame of atomic sphere approximation (LMTO-ASA) [3] and the VASP code using projector augmented-wave potential and plane basis set [4] are employed. Both methods are based on Density functional theory and the exchange and correlation contribution to the total energy was treated using generalized gradient approximation.

The calculated values B and a_0 agree well with available experimental data.

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