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THE LOSS OF MAGNETISM IN TETRAGONALLY DEFORMED Ni_3Al [1]

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We investigate changes of magnetic ordering in Ni_3Al in $L1_2$ structure along tetragonal (Bain's) deformation path. At some degree of deformation, the ferromagnetism of Ni_3Al is lost. We have determined phase boundaries between the magnetic and non-magnetic phases along the deformation path. Magnetic behavior of Ni_3Al was also investigated by means of Stoner model and by local environmental analysis, i.e. by investigating the number and type of atoms in the first coordination spheres.

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1 Introduction

The Ni-Al-based alloys possess many attractive properties for structural applications at elevated temperatures, such as high-temperature creep and excellent oxidation resistance. The Ni_3Al and other Al-based intermetallics exhibit anomalous yield behavior, that is, their yield strength increases rather than decreases with increasing temperature. Although single crystals of Ni_3Al are ductile, pure polycrystalline Ni_3Al is very brittle at room temperature because of grain-boundary fracture. The primary task of this contribution is to investigate changes of magnetic ordering in Ni_3Al along the tetragonal deformation path and to find phase boundaries between magnetic and non-magnetic phases.

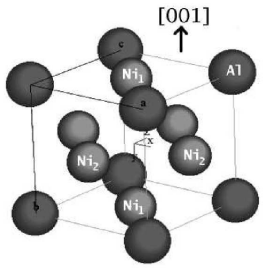

Fig. 1. The $L1_2$ structure of Ni_3Al.

2 Calculational Methods

The electronic structure calculations were performed by means of the full-potential linearized augmented plane wave (FLAPW) code WIEN, version 97 [1], based on the density functional theory. The results were obtained within the local density approximation (LDA) [2] for the

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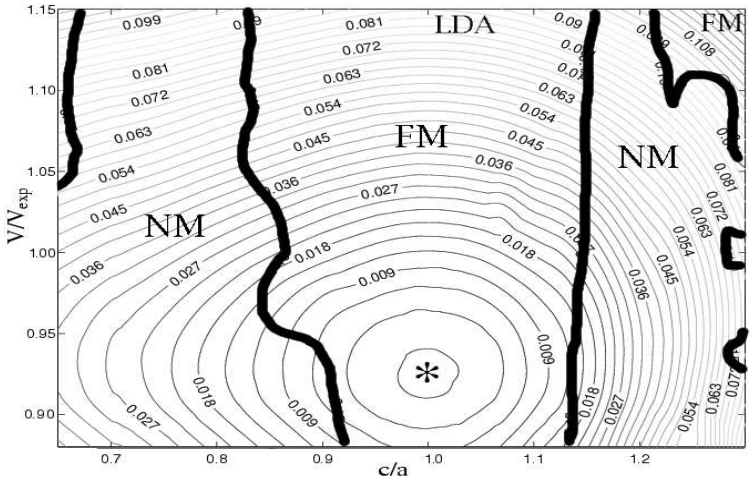

Fig. 2. The total energy (per formula unit) of Ni_3Al [Ry] calculated within the LDA as a function of volume (V/V_{exp}) and shape (c/a) deformation. The asterisk denotes the ground-state of Ni_3Al. For more details, see the text.

exchange-correlation term. Within this approximation the Stoner parameter does not strongly depend on volume [3]. In general, the displacive phase transformations between different high-symmetry structures could be simulated by some deformation paths that connect these structures. Here we investigate one of them, namely the tetragonal deformation path, often called Bain's path. It corresponds to an uniaxial deformation along the [001] direction while volume is kept fixed, and may be described by the c/a parameter, where c is measured along the deformation direction [001] and a is measured along a perpendicular direction. The $L1_2$ structure (Fig. 1) corresponds to $c/a = 1$. In this structure the Ni_1 and Ni_2 atoms are equivalent, but they become inequivalent when tetragonal deformation is performed.

3 Results and Discussion

We have calculated the total energy and magnetic moment of Ni_3Al with $L1_2$ structure along the tetragonal paths at cell volumes $V/V_{exp} \in 0.85 - 1.15$, where the V_{exp} is the experimental unit cell volume corresponding to the lattice constant $a = 3.568$ Å; the experimental magnetic moment is 0.23 μ_B per formula unit [4]. The zero total energy corresponds to the ground-state $L1_2$ structure of Ni_3Al, marked by an asterisk (Fig. 2) with the equilibrium lattice constant $a = 3.480$ Å and magnetic moment of 0.7 μ_B per formula unit. Employing the generalized gradient approximation for the exchange-correlation term yields the equilibrium lattice parameter $a = 3.561$ Å which is closer to the experimental value, but the magnetic moment is not changed too much (0.8 μ_B per formula unit [5]). It turns out that along tetragonal deformation path there is only one extremum of total energy, corresponding to the ground state. The thick lines from both sides of the ground state denote the phase boundaries between the non-magnetic (NM) and ferro-

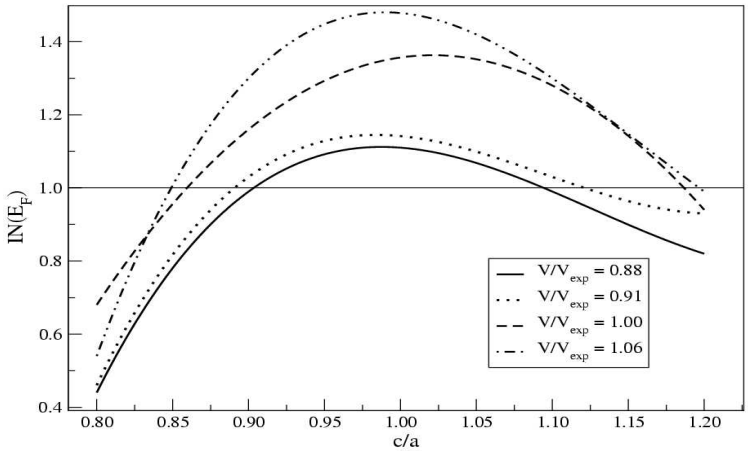

Fig. 3. The Stoner criterion for a few volumes along tetragonal deformation paths of Ni_3Al.

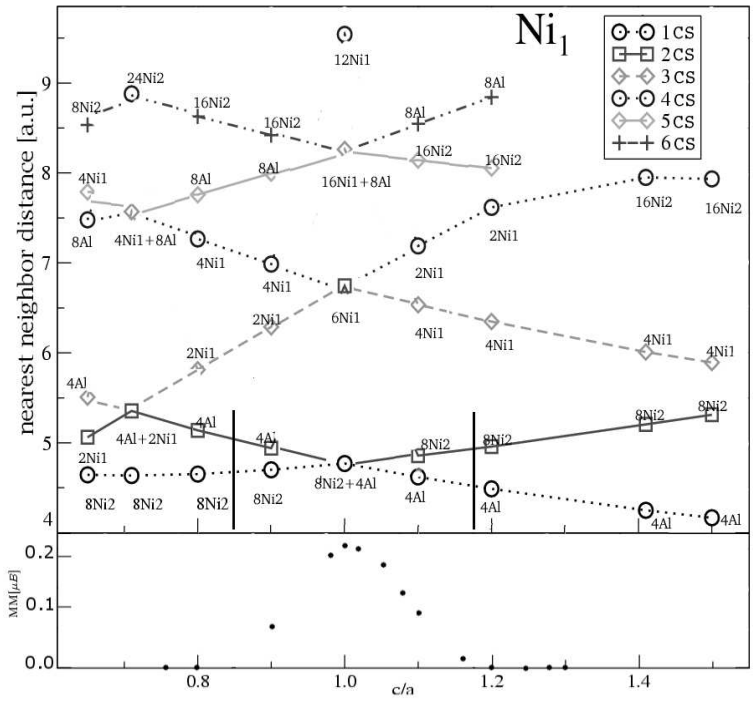

Fig. 4. The first six coordination spheres of Ni_1 atom site of Ni_3Al with $L1_2$ structure along the tetragonal deformation path. The lower panel of the figure shows the behavior of magnetic moment of Ni_1 atom. The results for Ni_2 atoms are similar.

magnetic (FM) regions. They are almost vertical, therefore the loss of the ferromagnetism does not depend on volume strongly. According to the well-known Stoner criterion the ferromagnetic ordering appears if $I\,N(E_F) \geq 1$, where I is the Stoner parameter and $N(E_F)$ is the paramagnetic density of states per spin at the Fermi level. The Stoner parameter for Ni_3Al in $L1_2$ structure was calculated to be 28.3 mRy [6]. We inspected Stoner criterion for a number of volumes along the tetragonal deformation path (Fig. 3) and the positions of phase boundaries agree very well with this criterion. Similarly we performed an analysis of local atomic environments in terms of number of neighbors, identification of different atomic species in the coordination spheres, and the relative distances between them (Fig. 4). In the $L1_2$ structure ($c/a = 1$), the atoms are in fcc positions. Each of them has 12 nearest neighbors and we observe maximum of the magnetic moment. However, during the tetragonal deformation the first coordination sphere splits (the nickel atoms become nonequivalent, see Fig. 1), and the magnetic moments will only survive for structures that partly resemble the original coordination. Fig. 4 shows that the magnetic behavior is only found if at least 8 atoms of nickel are present in the first two coordination spheres and the distance between the first and second coordination spheres does not exceed $0.054a_{L1_2}$, where a_{L1_2} is the lattice constant of $L1_2$ structure with the same cell volume as the deformed structure.

4 Conclusion

The phase boundaries between ferromagnetic and non-magnetic states were determined along the tetragonal deformation path of Ni_3Al in $L1_2$ structure. The origin of the magnetic behavior was analyzed by Stoner criterion and local environmental analysis. The ferromagnetic ordering occurs if at least 8 atoms of nickel are present in first two coordination spheres and their mutual distance does not exceed $0.054a_{L1_2}$.

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