

# Structural stability of NiAl with the $L1_0$ structure and local lattice distortion in the $Ni_3Al$ alloy around excess Al atoms

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## Abstract

For explaining asymmetry in the flow stress of  $Ni_3Al$  alloy as a function of aluminum content, the structural energy of ordered NiAl alloy with the  $L1_0$  structure is obtained with the electronic structure calculations based on the density functional theory. Quite a large distortion in the  $c$ -direction is found at the equilibrium, which means an  $L1_0$ -like local structure appearing in the Al-rich region of the  $Ni_3Al$  phase undergoes a large tetragonal strain. This tetragonal strain will give an explanation for the strengthening mechanism using the framework of Cocharadt et al. The effect of the Al concentration on the structural stability of  $L1_0$  in terms of the DOS is also discussed to explain the concentration dependence of the  $B2$ - $L1_0$  martensitic transition temperature.

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## 1. Introduction

The ordered  $Ni_3Al$  alloy is known to show an anomalous temperature dependence of the mechanical properties, i.e. it has higher flow stress at intermediate temperatures than at room or lower temperatures [1,2]. This property is very important in the industrial application and  $Ni_3Al$  is used mainly as precipitates in Ni-based superalloys for high-temperature structural applications.

Suzuki and his co-workers found that the flow stress of the  $Ni_3Al$  shows striking asymmetry around its stoichiometric composition: this compound shows a few times steeper increase of the 0.2% flow stress in the Al-rich compositions than in the Ni-rich compositions [3]. This tendency has also been confirmed by other researchers [4–6]. In the study of the solid solution strengthening in metals and alloys, the effect of local strain caused by the size mismatch between the matrix and alloying element has been taken to be the dominant factor. For the  $Ni_3Al$  alloy, however, there is no experimental observation of an

asymmetrical concentration dependence of the lattice constants between the Ni- and Al- rich portion [7]. Using the elastic theory Cocharadt et al. has found that the local tetragonal distortion in  $bcc$  iron caused by carbon interstitials considerably affects the motion of a dislocation [8]. Same kind of effects are expected for the Ni–Al system: in the Al-rich side of  $Ni_3Al$  phase the excess Al atoms locate at the neighboring site of Al in the  $L1_2$  structure implying the local configuration of  $L1_0$  structure in the  $L1_2$  structure as is shown in Fig. 1. If the  $L1_0$  NiAl has a tendency to show large tetragonal distortion at the equilibrium lattice constants without extra lattice volume change, the anisotropic strain yielded by the local  $L1_0$  configuration may explain the large enhancement of flow stress. Fig. 2 shows the Ni-rich portion of Ni–Al binary alloy phase diagram [9–11]. Although the NiAl alloy forms  $bcc$ -based  $B2$  structure, in the Ni-rich region  $B2$ -NiAl martensitically transforms into  $L1_0$  structure as has been reported by several researchers [11,12], which is the basis for the shape memory effect of this alloy. This suggests that the stability of NiAl with the  $L1_0$  structure is relatively high in the Al-rich compositions. Moreover, it is notable that  $Ni_5Al_3$  phase has  $L1_0$ -like structure.

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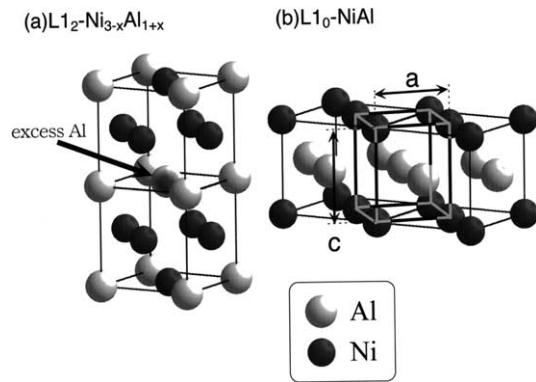


Fig. 1. (a) Local atomic configuration around excess Al atoms. The excess Al atoms locate at the Ni-sites and have 4 Al atoms as nearest neighbors. This local configuration is the same as that of the  $L1_0$ -structure. (b) Lattice structures for which the total energy was calculated. The base lattice has the  $fcc$  and  $bcc$  structures when the aspect ratio,  $c/a = \sqrt{2}$ , and 1, respectively.

The aim of this report is to present the structural energy data for the hypothetical  $L1_0$ -NiAl by the first-principles calculation and to explain the underlying physics of its stability. Though the electronic structure of  $L1_0$ -NiAl might be different for that of the  $L1_2$  system containing embedded anti-site Al atoms, the success of the cluster expansion approach by Conolly and Williams [13], where the energy of an alloy in an arbitrary atomic configuration is approximated by a sum of energies of atomic clusters seems to suggest the total energy of alloy is well approximated by a sum of local atomic configurations. The estimation of local lattice strain and asymmetry of flow stress will be given in a separated publication [14].

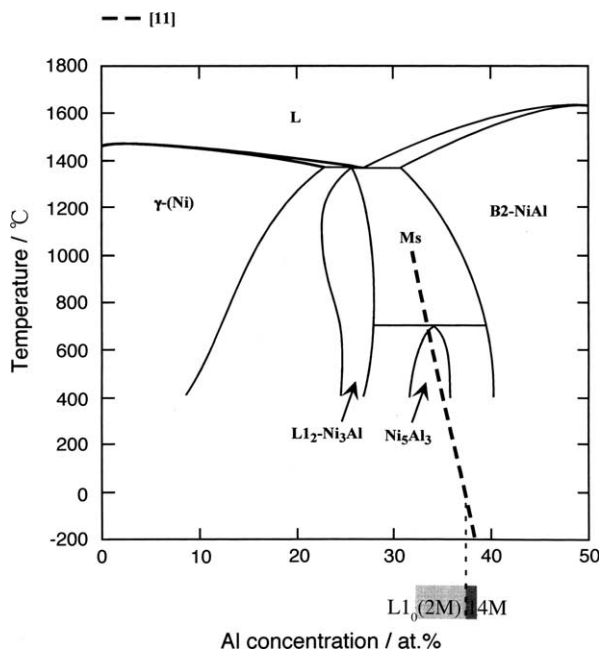


Fig. 2. Phase diagram of the Ni–Al system. The locus of martensitic transition temperatures from Ref. [11] is also drawn in this figure.

## 2. Computational procedure

The full-potential linearized augmented-plane-wave (FLAPW) method [15] was used for the energy calculations. The exchange-correlation potential parameterized by Moruzzi et al. [16] was used in the framework of density functional theory with local density approximation (LDA) [17]. For the  $k$ -space integration, 90 sampling  $k$ -points were taken in the irreducible wedge of Brillouin zone and cutoff wavelength was taken to be  $4.28 \text{ Bohr}^{-1}$  ( $8.09 \text{ \AA}^{-1}$ ), and cutoff angular momentum to be  $l_{\text{max}}=5$ . Atomic sphere radii at which the plane wave and spherical wave function are smoothly matched are fixed to  $2.100 \text{ Bohr}$  ( $1.111 \text{ \AA}$ ) and  $2.151 \text{ Bohr}$  ( $1.138 \text{ \AA}$ ) for Ni and Al, respectively. The electronic total energy was calculated for the alloy with the  $L1_0$  lattice structures for several lattice parameters,  $a$  and  $c$ , around the experimental unitcell volume.

## 3. Results and discussion

The calculated energy curves are shown in Fig. 3. First we fixed the  $c/a$ -ratio and varied  $a$  and  $c$ . Each energy curve has its minimum at a lattice constant,  $a_{\text{min}}(c/a)$ , and the energy,  $E(a_{\text{min}}(c/a))$ , has global minimum at  $c/a=1.00$ . The crystal structure at this global energy minimum has the  $B2$  structure, i.e.  $bcc$  based CsCl-type structure. The energy surface as functions of the volume and  $c/a$ -ratio is shown in Fig. 4. The energy takes a minimum at  $V=23.24 \text{ \AA}^3$  ( $156.8 \text{ Bohr}^3$ ) with  $c/a=1.00$ . The lattice constant at the minimum is  $a=2.85 \text{ \AA}$  while the experimentally measured lattice constant of the NiAl alloy in the  $B2$  structure is  $2.89 \text{ \AA}$ . Our result is consistent with the experimental

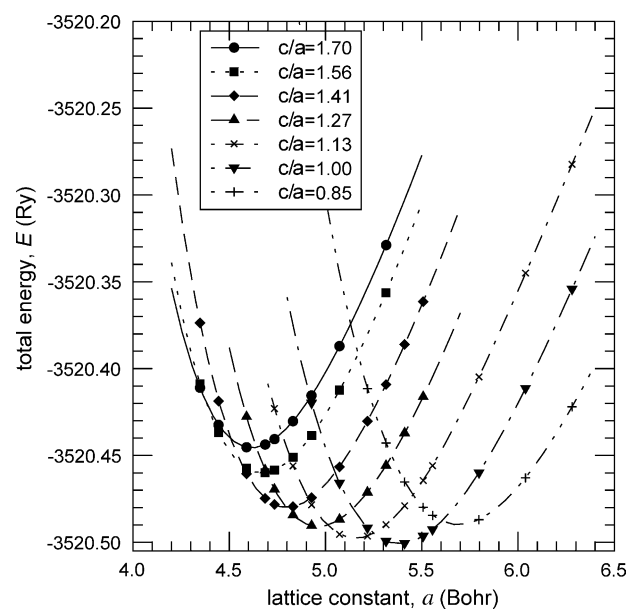


Fig. 3. Calculated total energy as a function of lattice constant,  $a$ . Energy curves for various aspect ratios,  $c/a$ , are shown.

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