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Surface structure and energy of B2 type intermetallic compound NiAl

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Abstract

The surface structure and energies for 22 surfaces of NiAl, an ordered intermetallic compound of B2 structure, have been studied by using embedded atom method. The results show that, for alternating Ni and Al surfaces with odd numbers of the sum of their three Miller indices, the energy difference between the Ni terminated surface and Al terminated surface increase linearly with increasing the interlayer distance. So from surface energy minimization, the Al terminated surface is favorable for each alternating Ni and Al surface. This is in agreement with experimental results. However, the energy of the (1 1 0) surface belonged to the other kind of the surface consisted of stoichiometric atomic layers and with even numbers of the sum of their three Miller indices, is the lowest in all two kinds of the surfaces. Therefore the (1 1 0) texture of NiAl appears mostly in the experiments.

Keywords: Intermetallic compound; NiAl; Surface structure; Surface energy; EAM

1. Introduction

NiAl is a well-ordered intermetallic compound with the B2 (CsCl prototype) structure, which consists of two interpenetrating simple cubic cells, where Al atoms occupy the cube corners of one sublattice and Ni atoms occupy the corners of the other sublattice. The properties of low density, good oxidation resistance and high yield strength have made B2-NiAl an attractive material for a wide range of engineering applications [1,2]. In recent years, there are many experimental [3–6] and theoretical [7–12] studies for the fundamental properties of NiAl. Such as point defects [7,8], dislocations [9], planar defects [10,11] and fractures [12,13]. A detailed knowledge of the structure and energy of crystal surfaces is important for the understanding of many surface phenomena such as adsorption, oxidation, corrosion, catalysis, segregation, reconstruction, crystal growth, etc. [14–17]. However, most investigations, from both experimental and theoretical side of view, are focused on the low-index surfaces [3,4,18–20].

In our previous papers, the surface energies for various orientations of the surface have been calculated for pure metals with FCC [21], BCC [22] and HCP [23] structures by using modified embedded atom method (MEAM) developed by Baskes et al. [24–26]. In this paper, the structures and energies have been studied and calculated for 22 surfaces of NiAl by using a reliable embedded-atom potential constructed by fitting to a large database of experimental properties and first-principles data of NiAl [27].

2. Computational methods

In the EAM [28], the total energy E_{tot} of a binary system is given by:

$$E_{\text{tot}} = \sum_i \left[F_{\alpha i}(\bar{\rho}_i) + \frac{1}{2} \sum_{j(\neq i)} \phi_{\alpha i - \alpha j}(r_{ij}) \right] \quad (1)$$

where the embedding energy $F_{\alpha i}(\bar{\rho}_i)$ represents the energy to embed an atom of chemical short α_i (=A or B) into the background electron density $\bar{\rho}_i$ at site i, $\phi_{\alpha i - \alpha j}(r_{ij})$ is a pair interaction between atoms i and j separated by a distance r_{ij}. The term in square brackets in Eq. (1) denotes the contribution to the

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total energy from the ith atom.

$$E_i = F_{\alpha i}(\bar{\rho}_i) + \frac{1}{2}\sum_{j(\neq i)} \phi_{\alpha i-\alpha j}(r_{ij}) \quad (2)$$

The following form of the embedding function is adopted [18],

$$F_{\alpha i}(\bar{\rho}_i) = a_1\bar{\rho}_i + a_2\bar{\rho}_i^{\,2} + a_3\bar{\rho}_i^{\,3} \quad (3)$$

where a_1, a_2, a_3 are fitting coefficients and $\bar{\rho}_i$ is the background electron density induced by all other atoms in the system.

$$\bar{\rho}_i = \sum_{j\neq i} \rho_{\alpha j}(r_{ij}) \quad (4)$$

Here the atomic electron density is given by:

$$\rho_{\alpha j}(r_{ij}) = s[r_{ij}^2 \exp(-\beta r_{ij}) + \varepsilon]\psi\left(\frac{r_{ij}-r_c}{h}\right) \quad (5)$$

where s, β, ε, r_c and h are parameters to be determined, and $\psi((r_{ij}-r_c)/h)$ is a cutoff function defined as:

$$\psi\left(\frac{r_{ij}-r_c}{h}\right) = \frac{((r_{ij}-r_c)/h)^4}{1+((r_{ij}-r_c)/h)^4} \quad (r_{ij}<r_c) \quad (6)$$

$$\psi\left(\frac{r_{ij}-r_c}{h}\right) = 0 \quad (r_{ij}\geq r_c) \quad (7)$$

The pair interaction potential $\phi_{\alpha i-\alpha j}(r_{ij})$ can be calculated by:

$$\phi_{\alpha i-\alpha j}(r_{ij}) = [DM(r_{ij}, r_0, \alpha, q) + \delta]\psi\left(\frac{r_{ij}-r_c}{h}\right) \quad (8)$$

where

$$M(r_{ij}, r_0, \alpha, q) = \exp[-q\alpha(r_{ij}-r_0)] - q\exp[-\alpha(r_{ij}-r_0)] \quad (9)$$

in which, D, r_0, α, q and δ are also fitting parameters. The form of the cutoff function guarantees that the atomic electron density and pair interaction potential turn smoothly to zero at the cutoff distance r_c, which is between the sixth and the seventh nearest neighbors.

Overall, there are seven potential functions involved in this model, which can be divided into three groups for convenience and simplicity: $\rho_A(r)$, $F_A(\bar{\rho})$, $\phi_{A-A}(r)$ describe atomic interactions in a pure-A system; $\rho_B(r)$, $F_B(\bar{\rho})$, $\phi_{B-B}(r)$ describe atomic interactions in a pure-B system and $\phi_{A-B}(r)$ describes pair interactions between unlike atoms A and B.

3. Surface structure of the B2-NiAl

For B2-NiAl, various surfaces are divided into two categories because surface structure depends on the surface orientation. If the sum of three surface indices $h+k+l$ is an even number, this kind of surface is of stoichiometric composition that each layer contains equal amounts of Ni and Al atoms and has one certain termination, such as the (1 1 0) surface. Otherwise, if $h+k+l$ is an odd number, this kind of surface has alternating Ni and Al layers which results in two different (Ni or Al) terminations, such as the (1 0 0) and (1 1 1) surfaces. Figs. 1 and 2 shows the surface configuration of two representative (1 1 0) and (1 0 0) surface, respectively.

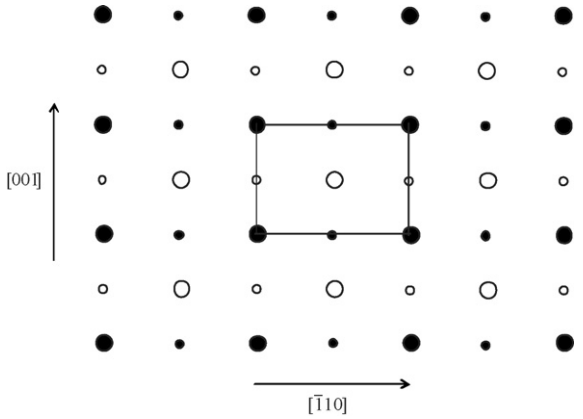

Fig. 1. Top-view of the NiAl (1 1 0) surface. Solid and blank circles represent Ni and Al atoms respectively. The larger and smaller circles indicate the atoms in the first and the second layers, respectively.

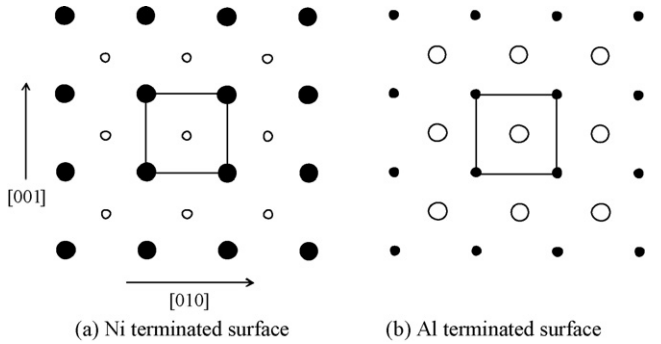

Fig. 2. Top-view of the NiAl (1 0 0) surface. (a) Ni termination, (b) Al termination.

In view of the contributions to the surface energy, many atomic layers should be included in the surface region while the atomic interactions extend to the sixth-nearest neighbors. In general, the higher the surface index is, the more atomic layers parallel to surface should be considered. Detailed analysis is given in the next section. Furthermore, according to the translation periodicity in surface plane, a minimum periodic cell should be selected in each surface. As shown in Fig. 1, a rectangle containing a Ni atom and an Al atom at each layer is chosen as a periodic cell for (1 1 0) surface and the other stoichiometric surfaces. For the (1 0 0) surface (Fig. 2) and the other Ni and Al alternating surfaces, a square containing a Ni atom or an Al atom at each layer is chosen as a periodic cell.

4. Calculation of the surface energy

The cohesive energy E_c of B2-NiAl equals to negative of the average value of the energy of a Ni atom in the bulk E_{Ni} and an Al atom in the bulk E_{Al} ($E_c = -(E_{Ni}+E_{Al})/2$), but the energy of a Ni or an Al atom at the surface is higher than that in the bulk. The energy difference summed over all atoms included in the periodic cell and then divided by the area of the periodic cell at the surface gives the surface energy density.