Physical behaviors of impure atoms during relaxation of impure NiAl-based alloy grain boundary

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Abstract The Monte Carlo simulation with the energetics described by the embedded atom method has been employed to mainly study physical behaviors of boron atoms during relaxation of the Ni_3Al-x at.% B grain boundary. During relaxation of impure Ni_3Al grain boundaries, we suggest that for different types of impure atoms(Mg, B, Cr and Zr atoms etc.), as the segregating species, they have the different behaviors, but as the inducing species, they have the same behaviors, i.e. they all induce Ni atoms to substitute Al atoms. Calculations show that at the equilibrium, when x(the B bulk concentration) increases from 0.1 to 0.9 , the peak concentration of B increases, correspondently, the peak concentration of Ni maximizes but the valley concentration of Al minimizes, at x = 0.5. The calculations also show the approximate saturation of Ni at the grain boundary at x = 0.5.

Keywords Grain boundary, Segregating species, Inducing species

CLC numbers O341, O552.2

1 Introduction

The intermetallic compound Ni_3Al has high strength at elevated temperature with a characteristic positive temperature dependence on strength over a certain temperature range.[1] Ni_3Al precipitate is extensively used as the γ′-strengthener in Ni-based superalloys,[2] but its brittle nature prevents Ni_3Al from being a structural material, despite the many attractive properties of the single crystal, such as low diffusivity and enhanced yield strength at high temperatures.[3] It has been demonstrated that addition of a small amount of B, Mg and Zr to Ni_3Al will remarkably improve its ductility.[4,5]

Using the embedded atom method(EAM), simulations of the effects of B[6] and Mg(or Zr)[7-9] on Ni_3Al grain boundaries have been performed by Chen *et al*.[6] and us,[7-9] respectively. We have shown not only that at the same zone, the Mg (or Zr)-induced distortion energy in the site of Al is always negative and lower than that of Ni, but also that the Mg (or Zr)-induced distortion energy in the Al site at the grain boundary is the lowest among those at all zones (the grain boundary,the bulk and the free surface). These might be one reason for Mg (or Zr) segregation being present with Al-depletion and Ni-enrichment at the grain boundary. Chen *et al*.[6] have found that the best cohesive properties of the Ni_3Al grain boundaries are obtained, when the boundary is Ni saturated and also with B present. Moreover, B and Ni cosegregate to the grain boundaries. Their finding[6] is very interesting and informative. For deep understanding of the B effects, very recently, we show how much amount of B is added to Ni_3Al for the boundary being Ni saturated, and also show how B and Ni cosegregate from the bulk to the boundary.[10] The purpose of present simulations is to give further explanations of the B and Mg effects, especially the B effect.

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2 EAM potential and Monte Carlo simulation

The EAM energy of an n-particle homonuclear system is given by

$$E = \frac{1}{2}\sum_{i\neq j}^{n}\phi(r_{ij}) + \sum_{i}^{n}F(\overline{\rho}_i) \qquad (1)$$

where E is the total energy of the system, r_{ij} is the distance between atom i and j, $\phi(r)$ is a pairwise interaction potential which is taken to be a Morse function, $F(\rho)$ is the embedding energy, and $\overline{\rho}_i$ is the electron density at atom i, which is contributed by its all neighbors.

Monte Carlo method was used to relax the grain structure to minimum energy configuration. There was a detailed explanation of MC simulation in Ref.[10].

3 Physical behaviors of B(or Mg) atoms during relaxation of Ni_3Al grain boundaries

Chen *et al*.[6] have shown that during relaxation of Ni_3Al-B grain boundaries, as the segregating species, the B atoms either insert into interstices in the grain boundary or substitute Ni atoms. Jiang *et al*. [8] have shown that during relaxation of the Ni_3Al-Mg grain boundaries, as the segregating species, the Mg atoms substitute either Al or Ni atoms(Note that the atomic radius for B, Ni, Al and Mg, equals 0.098 nm, 0.125 nm, 0.143 nm and 0.160 nm, respectively). Obviously, as the segregating species, B and Mg atoms have different behaviors during the relaxation of impure Ni_3Al grain boundary. Here, besides their different behaviors during the relaxation, we also suggest that as the inducing species, B and Mg atoms have the same behaviors, i.e. they all induce Ni atoms to substitute Al atoms.

To further clarify our opinion, the bulk effects of B on Ni_3Al grain boundaries will be analysed below in detail.

4 Bulk effects of B on Ni_3Al grain boundaries

Relaxation of the Ni_3Al-B system has been described by previous simulations[6] as follows: Starting with relaxed Ni_3Al-B grain boundaries, the B atoms either insert into interstices(the lowest density region) in the grain boundary or substitute Ni atoms. Subsequently, the grain boundaries are relaxed to the lowest energy. On the other hand, the measurements[4,5] have shown that when the B bulk concentration being 1 at.%, the grain boundaries are the Ni enrichment with B present, which can improve the cohesive properties of Ni_3Al. Evidently, the relaxation of the Ni_3Al-B system described by previous simulations[6] can not explain why the grain boundaries are the Ni enrichment with B present at the equlibrium, as found in the measurements,[4,5] because the substitution of B atoms into Ni sites is a negative effect on the Ni enrichment at the grain boundary, and the insertion of B atoms into interstices is a neutral effect on it. The above description does not involve any positive effect on it.

During the relaxation of the Ni_3Al-B system, as mentioned above, in our opinion,[10] starting with relaxed Ni_3Al-B grain boundaries, as the segregating species, the B atoms either insert into interstices in the grain boundary or substitute Ni atoms; meantime, as the inducing species, they induce Ni atoms to substitute Al atoms. Subsequently, the grain boundaries are relaxed to the lowest energy. According to our proposal, besides negative and neutral effects, the substitution of Ni atoms into Al sites induced by the B atoms, is a positive effect on the Ni enrichment at the grain boundary. This positive effect is the major cause of the Ni enrichment at the grain boundary. Therefore, our proposal might really explain the finding of the measurements mentioned above.[4,5]

5 Ni-saturation at the equilibrium for the Ni_3Al-0.5 at.% B grain boundary

How much amount of B is added to Ni_3Al for the boundary being Ni saturated?

Figs.2a-d of Ref.[10] have shown that for the Ni_3Al-x at.% B grain boundary, at x = 0.5 (Fig.2d of Ref.[10]), both the Ni-enrichment and the Al-depletion become the most obvious when x = 0.1→0.9. Also at x = 0.5, the Ni boundary concentration equals 97.5 at.% for -5-th layer, 98.2 at.% for 0-th layer and 96.0 at.% for 5-th layer, respectively. These three values are near 100 at.%, so there might be the approximate Ni-saturation between −5-th and 5-th layers of the boundary.

Fig.1 with accuracy shows the approximately symmetrical concentration profiles of Ni and Al, especially

the approximate Ni-saturation between -5-th and 5-th layers of the boundary.

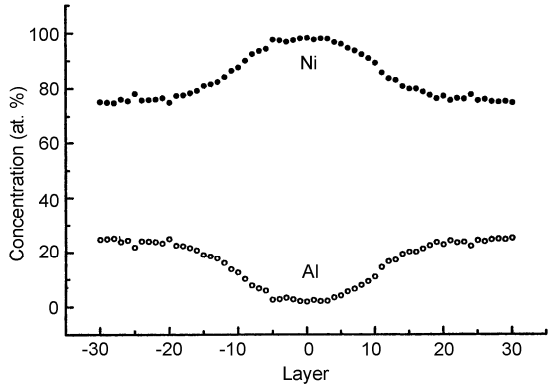

Fig.1 The simulated Ni(or Al) boundary concentration at the equilibrium for the Ni_3Al-0.5 at.% B [001]/Σ5(210)/36.87° symmetrical grain boundary.

Measurements[4,5] have shown that the best ductility(or cohesive properties) of Ni_3Al-B is obtained when its B bulk concentration equals 0.1 wt.% (i.e. about 0.45 at.%), .The simulations of Chen *et al.*[6] have found that the best cohesive properties of the Ni_3Al grain boundaries are obtained when the boundary is Ni saturated and also with B prasent, as metioned in Sec.1. Evidently, our present simulations(Fig.1) agree with the measurements[4,5] and the simulations of Chen *et al.* [6]

6 Peak and valley concentrations at the grain boundary plane

For the 100%Ni\100%Ni symmetrical grain boundary, at the equilibrium, Figs.2-3 of Ref. [10] have shown that the boundary concentration profiles of Ni, Al and B are approximately symmetrical with respect to the 0-th layer(the grain boundary plane). It is well known that in the boundary concentration profiles, the concentration data at the 0-th layer (the grain boundary plane) may be with the extreme value and generally either maximum or minimum, so they are indication of individual elements being either enriched or depleted at the grain boundary. There are definitions of peak and valley concentrations as follows: The concentration of an individual element at the 0-th layer (the grain boundary plane) is called the peak concentration if this element is enriched at the grain boundary, while the concentration is called the valley concentration if this element is depleted at the grain boundary.

A relation between the peak (or valley) concentration and *x* at.% (the B bulk concentration), might be interesting and available. Figs.2-3 show such a relation. Namely, when *x* increases from 0.1 to 0.5, the peak concentration of B increases from 3.4 at.% to 9.1 at.%; correspondently, the peak concentration of Ni increases from 83.2 at.% to 98.2 at.% while the valley concentration of Al decreases from 16.8 at.% to 1.8 at.%. Then, when *x* increases from 0.5 to 0.9, the peak concentration of B increases from 9.1 at.% to 14.7 at.%; correspondently, the peak concentration of Ni decreases from 98.2 at.% to 88.3 at.% while the valley concentration of Al increases from 1.8 at.% to 11.7 at.%. The phenomena can be attributed to that the positive effect dominates the Ni-enrichment and the Al-depletion at low B bulk concentrations, such as x = 0.1; while the negative effect dominates the Ni-enrichment and the Al-depletion at high B bulk concentrations, such as x = 0.9 as explained in Ref.[10].

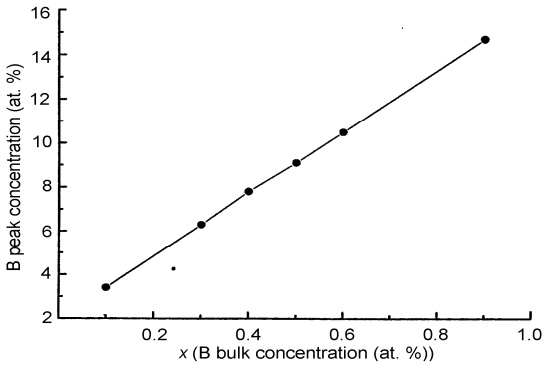

Fig.2 The B peak concentration at the grain boundary plane as a function of *x* (its bulk concentration) at the equilibrium for the Ni_3Al-0.5 at.% B [001]/Σ5(210)/36.87° symmetrical grain boundary.

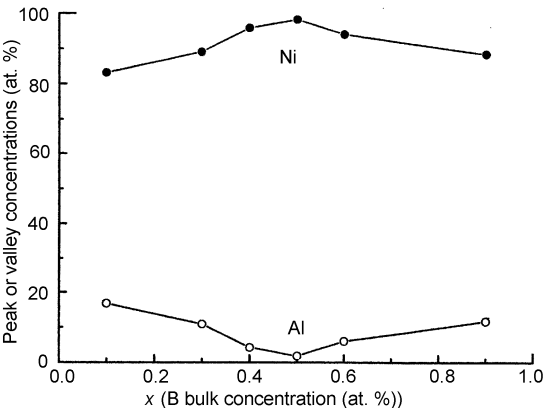

Fig.3 The peak(Ni) and the valley(Al) concentrations at the grain boundary plane as a function of *x* (the B bulk concentration) at the equilibrium for the Ni_3Al-0.5 at.% B[001]/Σ5(210)/36.87° symmetrical grain boundary.

7 Summary

The embedded atom method (EAM) is used to calculate peak concentrations of Ni and B, and valley concentration of Al, at the Ni_3Al-*x* at.% B (100%Ni\100%Ni) [001]/∑5(210)/36.87° grain boundary at the equilibrium. Calculations show that when *x* (the B bulk concentration) increases from 0.1 to 0.9, the peak concentration of B increases, correspondently, the peak concentration of Ni maximizes but the valley concentration of Al minimizes, at $x = 0.5$. The calculations also show the approximate saturation of Ni at the grain boundary at $x = 0.5$, in detail. We emphasize that for different types of impure atoms (Mg, B, Cr and Zr atoms etc.), as the segregating species, they have different behaviors, but as the inducing species, they have the same behaviors, i.e. they all induce Ni atoms to substitute Al atoms.

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