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Simulations of Bulk Effects of Zr on Cohesion of Ni_3Al Grain Boundary*

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摘 要: Monte Carlo simulation with the energetics described by the embedded atom method has been employed to calculate dependence of the grain boundary cohesion on the Zr bulk atom concentration, for the Ni_3Al-x % Zr (100%Ni\100%Ni)[001]/Σ5(210)/36.87° symmetric tilt grain boundary, at the equilibrium. Calculations show that when x (the Zr bulk atom concentration) increases from 0.1 to 0.5, the Zr enrichment increases, both the Ni enrichment and the Al depletion maximizes at $x = 0.3$. The calculations also show the best cohesion of the grain boundary at $x = 0.3$.

Key words: grain boundary concentration; inducing and segregating specie; bulk effect

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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]. This remarkable property, however, is not sufficient to make it useful for high-temperature applications because of its brittleness and unfabricability. It has been demonstrated in experiments that the addition of a small amount of B, Cr, Mg or Zr (trace element) to Ni_3Al remarkably improves its ductility[1－9].

Quantitative dependence of the cohesive properties of the Ni_3Al grain boundaries (or ductility of Ni_3Al) on the bulk concentration of the trace element has been studied for years. For example, for the Ni_3Al-B system, the measurements[3] and the simulations[4, 5, 9] have shown that the cohesive properties of the Ni_3Al grain boundaries will be improved when its B bulk atom concentration is below about 1 %, and also that the best cohesive properties of the Ni_3Al grain boundaries will be obtained when its B bulk atom concentration equals about 0.5 % (weight fraction 0.1 %). However, for the Ni_3Al-Zr system, to our knowledge, this dependence has been not studied until now. The aim of present simulation work studies such dependence. The simulation method is the Monte Carlo one conjoined with the embedded atom method (EAM) po-

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tentials[4—9].

2 EAM Potentials and Monte Carlo Simulation

2.1 Potentials

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

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

where E is the total energy of the system, r_{ij} is the distance between atom i and j, and $\phi(r)$ is a pairwise interaction potential which is taken to be a Morse function, $F(\rho)$ is the embedding energy and $\bar{\rho}_i$ is the electron density at atom i, which is contributed by it's all neighbors. For the Ni_3Al-Zr system, the optimized potential parameters are adopted from Ref. [8].

2.2 Monte Carlo simulation

Monte Carlo method is used to relax the grain structure to the lowest energy configuration at the room temperature (25℃). The unrelaxed, starting structure of the grain boundary is assumed to be the coincidence site lattice (CSL) model. The (100%Ni\100%Ni)[001]/Σ5(210)/36.87° symmetric tilt boundary structure of Ni_3Al is chosen.

A schematic drawing of the computation cell is shown in Fig. 1 of Ref. [5]. The initial bulk concentration of Zr atoms in the computation cell is given as x atoms % (x= 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9 and 1.0), and this concentration disperses randomly homogeneously. The present results in Sect. 3 are statistical (average of a few million MC steps per atom after equilibrium) for each system of 82 620 atoms.

3 Results and Discussion

3.1 Definition of the bulk effects of Zr

Starting with relaxed Ni_3Al-Zr grain boundary, as the segregating species, the Zr atoms substitute either Al or Ni atoms[8]; in our opinion, meantime, as the inducing species, the Zr atoms induce Ni atoms to substitute Al atoms. Subsequently, the grain boundary is relaxed to the lowest energy. Thus, the bulk effects of Zr on the grain boundary include the primarily positive effect on the Ni enrichment at the grain boundary, the secondarily positive effect on it, and the negative effect on it. The primarily positive effect is defined as the Zr atoms inducing Ni atoms to substitute into Al sites, the secondarily positive effect is defined as the Zr atoms substituting into Al sites, and the negative effect is defined as the Zr atoms substituting into Ni sites.

3.2 Analysis of the bulk effects on boundary concentrations

For the Ni_3Al-x atoms % Zr (100%Ni\100%Ni)[001]/Σ5(210)/36.87° symmetrical tilt grain boundary, at the equilibrium, Fig. 1 shows that when x (the Zr bulk concentration) increases from 0.1 to 0.5, the Zr enrichment increases, both the Ni enrichment and the Al depletion maximizes at x =0.3.

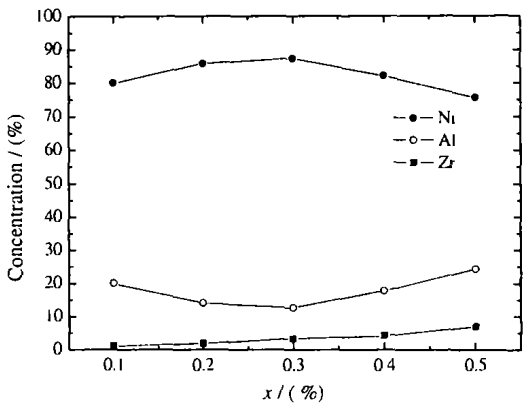

Fig. 1 The atom concentrations of Zr, Ni and Al as a function of x (the Zr bulk atom concentration) at the equilibrium for the Ni_3Al-x % Zr [001]/Σ5(210)/36.87° symmetrical grain boundary.

For relaxation of the Ni_3Al-x atoms % Zr grain boundary, in our opinion, the primarily positive effect is main cause of the Ni enrichment at the grain boundary, the secondarily positive effect plays an "enhancing" role; but the negative effect

plays a "weakening" role, especially at high Zr bulk concentrations such as $x=0.5$, where this negative effect becomes strong, because the significant Zr enrichment (Fig. 1) is formed by the 100% Zr atoms substituting into Ni sites (Fig. 2).

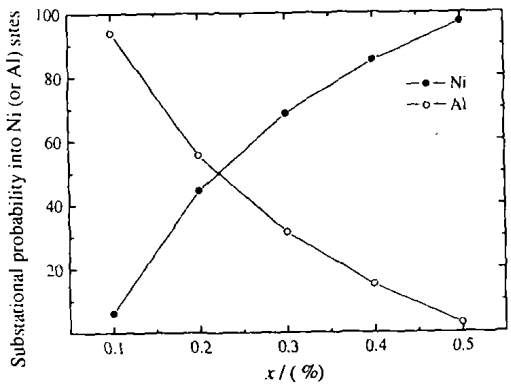

Fig. 2 The substitutional probability of Zr atoms into Al (or Ni) sites as a function of x (the Zr bulk atom concentration) at the equilibrium for the Ni_3Al-x % Zr [001]/Σ5(210)/36.87° symmetrical grain boundary.

Also in our opinion, study of combination of the positive and the negative effects is available, in order to understand the dependence of the cohesive properties of Ni_3Al grain boundaries on the Zr bulk concentration, particularly in order to search the Zr bulk concentration corresponding to the best cohesive properties of Ni_3Al grain boundaries.

According to the above explanations, for the Ni_3Al-x % Zr grain boundary at the equilibrium, at low Zr bulk concentrations, such as $x=0.1$, due to the positive effects, corresponding to the Zr enrichment increasing, the Ni enrichment and the Al depletion increase (Fig. 1). However, at high Zr bulk concentrations, such as $x=0.5$, due to the negative effect, corresponding to the Zr enrichment increasing, the Ni enrichment and the Al depletion decrease (Fig. 1). Therefore, between low ($x=0.1$) and high ($x=0.5$) Zr bulk concentrations, there might be a Zr bulk concentration, at which the Ni enrichment and the Al depletion maximize ($x=0.3$(Fig. 1)).

3.3 Analysis of the bulk effects on cohesive properties

As shown in Fig. 1, for the Ni_3Al-x % Zr grain boundary, at the equilibrium, when x (the Zr bulk concentration) increases from 0.1 to 0.5, the Zr enrichment increases, both the Ni enrichment and the Al depletion maximizes at $x=0.3$. Are the best cohesive properties of the Ni_3Al-x % Zr grain boundary obtained at $x=0.3$? Calculations of the Griffith grain boundary cohesion energy ($\gamma_{coh,\ for\ GB\ (210)}$) and the bulk one ($\gamma_{coh,\ for\ bulk\ (210)}$) are necessary to answer this question[9].

For the Ni_3Al-x % Zr (210) bulk, the present calculations show that $\gamma_{coh,\ for\ bulk\ (210)}$ ($\leqslant 4\ 327$ mJ/m^2 in the range of $x=0.1$—0.5, i. e., its relative change is always less than 0.5 % ($-0.5\ \% < (1-\gamma_{coh,\ for\ bulk\ (210)}/4\ 327\ mJ/m^2) \times 100\% < 0.5\ \%$) when x changes between 0.1 and 0.5. For the Ni_3Al-x % Zr (210) grain boundary, the present calculations show that $\gamma_{coh,\ for\ GB\ (210)}/\gamma_{coh,\ for\ bulk\ (210)} > 0.79$ in the range of $x=0.1$—0.5, and its best value is 0.89 at $x=0.3$, i. e., the best cohesion of the grain boundary is obtained when $x=0.3$(Fig. 3). Note that for the Ni_3Al grain boundary (210), $\gamma_{coh,\ for\ GB\ (210)}/\gamma_{coh,\ for\ bulk\ (210)}=0.73$.

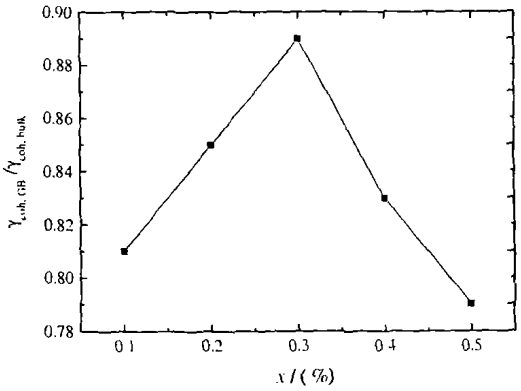

Fig. 3 The Griffith cohesive energy ratio of the GB (grain boundary) to the bulk, i. e. $\gamma_{coh,\ for\ GB}/\gamma_{coh,\ for\ bulk}$, as a function of x (the Zr bulk concentration) for the Ni_3Al-x % Zr [001]/Σ5(210)/36.87° symmetrical grain boundary.

4 Conclusion

Monte Carlo simulation with the energetics described by the embedded atom method (EAM)

has been employed to calculate not only grain boundary concentrations of Ni, Zr and Al, but also dependence of the grain boundary cohesion on the Zr bulk concentration, for the Ni_3 Al-x % Zr (100%Ni\100%Ni)[001]/Σ5(210)/ 36.87° symmetric tilt grain boundary, at the equilibrium. The calculations show that when x (the Zr bulk atom concentration) increases from 0.1 to 0.5, the Zr enrichment increases, both the Ni enrichment and the Al depletion maximizes at $x=0.3$. The calculations also show the best cohesion of the grain boundary at $x=0.3$.

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模拟锆(Zr)的基体效应对 Ni_3Al-x atoms % Zr 晶界内聚性的影响*

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摘　要: 利用双粒子模型研究微量元素锆(Zr)的基体效应对 Ni_3Al-x atoms % Zr 晶界内聚性的影响. 模型显示, x[锆(Zr)的基体浓度]从 0.1 增加到 0.5, 在晶界 Zr 富集是增加的; Ni 富集和 Al 贫乏在 $x=0.3$ 时趋于最大. 模型还显示, Ni_3Al-x atoms % Zr 晶界的内聚性在 $x=0.3$ 时为最佳.

关 键 词: 晶界浓度; 偏析子与诱发子; 基体效应

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