MOLECULAR STATIC SIMULATION OF ENERGY FEATURES OF INTERACTION BETWEEN GRAIN BOUNDARY AND DISLOCATIONS IN Ni_3Al ALLOY①

Chen, Da Lu, Min Lin, Dongliang
Department of Materials Science, Shanghai Jiao Tong University, Shanghai 200030

ABSTRACT

The molecular static relaxation method has been used to simulate the energy features of the interaction between the grain boundary(GB) and dislocations in Ni_3Al alloys. The effects of various factors, such as the GB chemistry, the dissociation type of superdislocation, the geometrical index of the GB, boron segregation and an applied stress on the energy feature of the interaction have been studied. Their relations with the mechanical behavior of the GB and mechanism responsible for boron-enhanced ductility have also been discussed.

Key words: Ni_3Al Intermetallics grain boundary structure dislocation computer simulation

1 INTRODUCTION

The intermetallic compound Ni_3Al, which has a high potential for structural applications at elevated temperatures, shows intrinsic intergranular brittleness in polycrystalline forms. The segregation of a small amount of boron at grain boundaries(GBs) can significantly increase the ductility of Ni_3Al at ambient temperature. However, only in a slightly Ni-rich alloy will the boron has ductilizing effect. The GB is normally considered as the obstacle to the dislocation motion and also as the source and sink of dislocations. Therefore, the interaction between the GB and dislocations will greatly affect the deformation and fracture features of the material. In our previous works[1-5], simulative studies have been carried out on the atomistic structures and their energy characteristics of different GBs with Ni-rich, Al-rich and stoichiometry GB chemical compositions in the both cases of with and without boron segregation. In this paper, the atomistic simulation method has been used to further study the interaction between the GB and dislocations in Ni_3Al from the viewpoint of its energy feature, including the effects of various factors, especially the boron segregation and GB chemistry, on the interaction. This will be helpful to the better understanding of the reason for the intrinsic brittleness and mechanism responsible for boron-enhanced ductility in Ni_3Al.

2 SIMULATION PROCEDURE

The interaction between atoms was described using potentials related to the embedded atom method(EAM), and a molecular static(MS) relaxation method combined with a steepest decent computational technique was used in the simulation. Starting from an initial GB configuration which was constructed using the coincidence site lattice (CSL) model, the GB structure was first relaxed[1-5], then the relaxed GB with the lowest energy was used as a starting configuration for the GB-dislocation relaxation.

The different GB compositions were obtained by withdrawing different atomic layers parallel to

① Received Oct. 20, 1993

the boundary plane so as to make the atomic layer at the boundary plane have the Al/Ni atomic ratio being equal to, larger or smaller than 1/3 (corresponding to stoichiometry, Al-rich or Ni-rich GB respectively). Meanwhile, the same atomic layers which have been withdrawn at the boundary region were added to the out region of the computational block according to the periodicity of the crystal lattice. The experimental result shows that only a slight variation (about 0.5 at.-%～1.0 at.-%) of bulk aluminum content will intensely influence the beneficial effect of boron segregation on the ductility, while the corresponding variation of aluminum content at the GB is much larger than that in the bulk[6]. Therefore, the main factor to affect the ductilizing effect of boron is the GB composition. The method mentioned above to obtain different GB compositions will not change the composition outisde the GB region, i. e. it still keeps the bulk with a stoichiometric composition, which is approximately in accord with the chemistry situation of the Ni_3Al alloy in practical use. Besides, while simulating the GB with boron segregation, boron atoms at the GB were placed in the center of the polyhedrons with the larger size and at where the boron atoms will have the lower energies.

The introduction of a superdislocation to be simulated was accomplished by imposing a suitable strain field on all atoms according to the elastic theory of dislocation. One of the dissociated superpartials (leading superpartial), which is parallel to the tilt axis of GB $[\bar{1}01]$, was positioned near the GB (less than the cut-off radius of the potential) and at where the superpartial has the lowest energy. The other superpartial (trailing superpartial) was located at the other side of a fault (APB or SISF) outside the computational block, and its effect on the leading superpartial and GB was taken into account by imposing an additional elastic strain field caused by that superpartial.

The distance between these two superpartials was determined by using the elasticity theory and the given fault energy. The relaxed GB structure plus the elastic strain field of a superdislocation made up the starting configuration for the simulation of GB-dislocation interaction. The dimension of the computational block for the relaxation in the two normal directions perpendicular to the tilt axis was chosen as at least three times of the cut-off radius of the potential, while in the direction of the tilt axis the lattice periodicity was used so that the block was effectively infinite in this direction.

The effect of an applied stress on the dislocation core structure and its interaction with the GB was considered by imposing upon the block a homogeneous shear strain corresponding to the shear stress. The shear stress was always applied in the direction of Burgers vector $[\bar{1}01]$, which will lead to the extension of the distance between two superpartials, i. e. it will force the leading superpartial to move towards the GB plane.

In this work, four types of GBs, namely $\Sigma3(111)$, $\Sigma3(121)$, $\Sigma11(131)$ and $\Sigma27(151)$ GBs with the $[\bar{1}01]$ tilt axis were chosen. Among them $\Sigma13(121)$ and $\Sigma27(151)$ GBs were further divided into Ni-rich and Al-rich GBs. On the other hand, in $L1_2$ ordered alloys, the dissociation of a superdislocation is very complex due to the anisotropic energy of crystalline planes resulted from the compositional differences between these planes. Of the possible dissociations, the following three types of dissociations, which are related to the deformation behavior and also favorable from the energy consideration in Ni_3Al, were ued in the present study[7]:

(111)APB, (010)APB
$\{[\bar{1}01]=1/2[\bar{1}01]+1/2[\bar{1}01]\}$ and
(111)SISF
$\{[\bar{1}01]=1/3[\bar{2}11]+1/3[\bar{1}\bar{1}2]\}$

3 RESULTS AND DISCUSSION

If a dislocation is introduced in the vicinity of a GB, the GB structure and the dislocation core structure will be altered because of their interaction[8-10]. It, therefore, can be expected that their interaction will also be reflected in the variation of GB energy. Table 1 gives ratios of GB energies for the four types of GBs with and without a dislocation close to them (E_{gbd}/E_{gb}), under the various conditions of three types of superpartial dissociations, different GB compositions, with and without boron segregation. It can be more clear to show the GB energy variation due to the introduction of a dislocation by using the energy ratio E_{gbd}/E_{gb} than by

Table 1 E_{gbd}/E_{gb} **values at different conditions, where** E_{gbd} **and** E_{gb} **represent the GB energy after and before the introductions of a superdislocation to the vicinity of the GB respectively.** Ni_R, Al_R **and Sto. correspond to the Ni-rich, Al-rich and stoichiometry GB respectively.** B_F **and** B_D **represent the boron-fee and boron-doped GB respectively.**

		Ni_R, B_F	Al_R, B_F	Ni_R, B_D	Al_R, B_D	Sto., B_D	
(111)APB	Σ3(121)	1.195	1.351	1.002	1.030	Σ3(111)	0.947
	Σ27(151)	1.245	1.398	1.032	1.038	Σ11(131)	1.018
(111)SISF	Σ3(121)	1.195	1.449	1.017	1.023	Σ3(111)	0.946
	Σ27(151)	1.269	1.513	1.059	1.031	Σ11(131)	1.034
(010)APB	Σ3(121)	1.140	1.264	1.011	1.031	Σ3(111)	0.982
	Σ27(151)	1.201	1.136	0.998	1.001	Σ11(131)	1.010

using the GB energies(E_{gbd} and E_{gb}) directly.

The interaction energies between the GB and dislocation, which is defined as $E_{int} = E_{gbd} - (E_{gb} + E_{dis})$, are listed in Table 2. The effect of an applied stress on the GB(plus a dislocation) energy in the boron-free and boron-doped cases are given in Table 3.

Table 2 The interaction energy between the GB and dislocation $E_{int} = E_{gbd} - (E_{gb} + E_{dis})$, **where** E_{dis} **represents the energy of the dislocation.**

	(111)APB	(111)SISF	(010)APB
Σ3(111)	−144	−18	−195
Σ3(121)	−325	−232	−306
Σ11(131)	−299	−270	−256

From Table 1 it can be seen that the GB energy will increase when a dislocation is introduced nearby the GB. Its increment varies depending on the type of dissociation, the GB chemistry and the GB geometrical index. Generally, the increment of energy in the Ni-rich GB is lower than that in the Al-rich GB. Besides, the increment is the largest for the (111)SISF dissociation and smallest for the (010)APB dissociation. This could be caused by the reason that apart from the same screw component of the superpartial in the (111)APB dissociation, there is an additional edge component of the superpartial in the (111)SISF dissociation, thus the interaction between the dislocation and GB becomes stronger and then it makes the energy higher for the (111)SISF dissociation. Among the four types of GBs studied, the introduction of a dislocation near the GB has a smallest effect on the GB energy for the Σ3(111) GB, while the increment of GB energy is largest for the Σ27(151) GB.

The most important result is that with the boron segregation there will be almost no increase of the GB energy when a dislocation is introduced in the vicinity of a GB, and even a slight decrease for the Σ3(111) GB. Moreover, the increments of GB energy are lower in Ni-rich GBs than those in Al-rich GBs, which agrees with the other simulation result that, with the boron addition, the GB energy is much lower in the Ni-rich GB than in the Al-rich GB[1-5]. This also demonstrates the ductilizing effect of boron on the Ni-rich GB, because the cohesive energy of a GB is in inverse proportion to the GB energy.

Table 2 shows that all the E_{int} values are negative, which means that the movement of dislocations from interior of the grains to GBs is favorable from an energy viewpoint. When under the applied stress, dislocations will move towards the GB by overcoming various moving resistances, then dislocations will be absorbed by the GB. Because the existence of a dislocation will result in the distortion of crystal lattice, the dislocation situated at the GB, where the atomic arrangement is more loose than that in the bulk, is more suitable or stable than that within the grain. Only when the applied

Table 3 E^{S}_{gbd}/E_{gbd} **(boron-free) and** $E^{S,B}_{gbd}/E^{B}_{gbd}$ **(boron-doped) values of Ni-rich Σ3(121) GB, Ni-rich and Al-rich Σ27(151) GBs at various applied stresses, where** G **is the shear modules; superscripts S and B represent the applied stress and boron addition, respectively.**

	E^{S}_{gbd}/E_{gbd}					$E^{S,B}_{gbd}/E^{B}_{gbd}$			
	Σ3(121)			Σ27(151)		Σ3(121)		Σ27(151)	
		Ni-rich		Ni-rich	Al-rich	Ni-rich		Ni-rich	Al-rich
	0.02G	0.04G	0.06G	0.04G	0.04G	0.04G	0.06G	0.04G	0.04G
(111)APB	1.074	1.169	1.154	1.275	1.388	1.042	0.991	1.033	1.146
(111)SISF	1.049	1.114	1.146	1.297	1.402	1.005	1.003	1.067	1.175
(010)APB	1.049	1.157	1.141	1.258	1.373	1.005	0.988	1.014	1.026

stress is large enough, will dislocations be emitted from the GB into the neighboring grain, otherwise, dislocations will pile up at the GB. Thus, the magnitude of E_{int} reflects the degree of stability of the dislocation situated at the GB or the degree of ease for the GB to emit dislocations.

The interaction energy is also affected by the GB geometrical index. For the three types of GBs simulated, the absolute E_{int} value of Σ3(111) GB is smallest as compared with those of Σ3(121) and Σ11(131) GBs. This implies that in the case of Σ3 (111) GB, when a dislocation locates at the GB or within the grain, their energy difference is smallest. Therefore, the ability of GB to absorb and emit dislocations is much higher. While for the other two GBs, dislocations have a high tendency to locate at GBs and thus they are more difficult to spread into the neighboring grain. These simulation results of the GB energy and the interaction energy explain, from the energy consideration, the experimental phenomenon that Σ3(111) GB has a rather high resistance to the intergranular fracture in Ni_3Al[11].

The GB energy of a Ni-rich Σ3(121) GB increases with increasing applied stress up to 0.04G (see Table 3). This is because, with increasing the stress the leading superpartial tends to move towards the GB, then the interaction between the dislocation core and a GB becomes stronger, which results in an increase in the GB energy. However, when the stress is increased to 0.06G, the GB energies in the cases of (111)APB and (010)APB dissociations do not increase further, rather they decrease slightly. This indicates that, when the stress exceeds a critical value, the extension of the core structure may pass through the GB in order to release the stress concentration. While in the case of (111) SISF dissociation the GB energy increases further when the stress is increased to 0.06G, which means that compared with other two dissociations the core structure of superpartial in the (111) SISF dissociation is more difficult to extend across the GB.

The most striking feature of the GB with boron segregation is that, when the stress is applied, there is almost no change of GB energy (at a stress of 0.04G) and even a slight decrease (at a stress of 0.06G) compared with the GB energy in the case of boron-doped but without the applied stress. This further demonstrates the fact that, with the help of boron segregation and under an applied stress, the ability of a dislocation to extend across the GB is significantly increased in the Ni-rich GB, which is also confirmed by the simulation study of the dislocation core structure in the GB rgion[8-10].

The situation of the Σ27(151) GB is quite similar to that observed in the Σ3(121) GB (also shown in Table 3). The only difference between them is that the Σ27(151) GB has a slight higher resistance to the core spreading across the GB than the Σ3(121) GB does. This is because the atomic environment of the GB region within which the dislocation lying on varies with the GB geometrical index, thus the interaction between the GB and a dislocation will be different. Meanwhile, for the Σ27(151) GB the effect of GB composition is also

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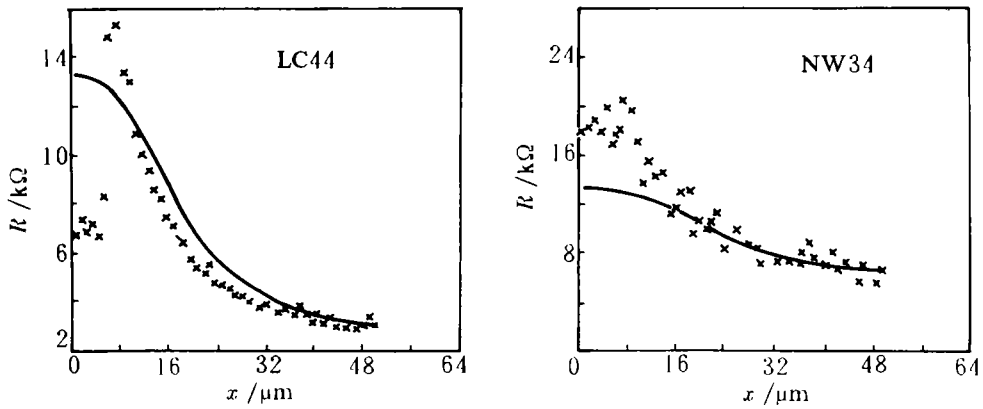

Fig. 5 Comparison of calculated curve(—)according to error equation with experimental curve(XXX)

4 RESULTS

Vertical distribution of oxygen after outdiffusion can be described in form of series equation (3).

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obvious. When a superpartial moves towards the GB under an applied stress, the increase of GB energy is obscure, especially for the boron-doped Ni-rich GB.

4 CONCLUSIONS

(1) The segregation of boron lowers the energy barrier needed to be overcome to the absorption and emission of dislocations at the GB, which eases the release of stress concentration caused by the pile-up of dislocations at the GB and reduces the tendency of intergranular fracture.

(2) The effect of boron to lower the energy barrier is more pronounced in Ni-rich GBs than in Al-rich GBs. The Σ3(111) GB behaviors the lowest energy barrier to the dislocation motion. The (111)SISF superdislocation dissociation is more unfavorable, from an energy viewpoint, to the dislocation motion in the GB region than the (111)APB and (010)APB dissociations.

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