Creep and fatigue damages of Ni-base- superalloy caused by strain-induced anisotropic diffusion of component elements

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Abstract. The mechanism of the directional coarsening of γ' phases (rafting) of Ni-base superalloy under an uni-axial strain was analyzed by molecular dynamics (MD) analysis. The stress-induced anisotropic diffusion of Al atoms perpendicular to the interface was observed clearly in a $Ni(001)/Ni_3Al(001)$ interface structure, The reduction of the diffusion of Al atoms perpendicular to the interface is thus, effective for improving the creep and fatigue resistance of the alloy. It was also found that the dopant elements in the superalloy also affected the strain-induced diffusion of Al atoms. Pd was one of the most effective elements which restrain Al atoms from moving around the interface.

Introduction

Ni-base superalloys have been widely applied to gas turbine blades in combustion power plants and aircraft engines. Directionally solidified Ni-base superalloys are mainly employed for the blade material used at high temperatures because they show the superior stress-rupture resistance, higher thermal fatigue resistance, and higher incipient melting temperatures comparing with the polycrystalline Ni-base superalloys. The strength of the Ni-base superalloys at high temperatures is improved by the fine cuboidal γ' phase (Ni_3Al) orderly-dispersed in a $\gamma\square$ phase (Ni-rich matrix) because the fine texture in a grain prevents dislocations from moving in the grain easily. However, directional coarsening of the γ' phase perpendicular to a principal stress, which is called "rafting," has been found to occur when an uni-axial external stress is applied to the superalloys at high temperatures. The morphological change of the directionally solidified Ni-base superalloy (CM247LC) observed during a creep test at 1173 K [1,2] is summarized in Fig. 1. The magnitude of the uni-axial stress applied to the specimens was fixed at 216 MPa during the test. Since the direction of the uni-axial load in this figure is up and down, the rafting proceeded along the horizontal direction of this figure, which is perpendicular to the direction of the applied load. The average size of the initially dispersed γ' phase was about a few hundred nm. With increasing the loading time, the γ' phase starts to grow perpendicularly to the direction of the applied load, and the initial finely-dispersed texture changed to a large layered texture as shown in Fig. 1. Similar micro texture change was observed in this alloy after fatigue loading [3]. Once the layered texture appears, the strength of the alloy at high temperatures decreases drastically and cracks starts to propagate rapidly along the layered interface between the γ' and γ phase and thus, creep fracture is accelerated seriously. Therefore, it is very important to clarify the mechanism of the rafting for improving the strength of the Ni-base superalloy at high temperatures under the applied load and thus, assuring the reliability of the turbine systems. In this study, in order to make clear the mechanism of the rafting, the strain dependence of diffusion characteristics of component elements in Ni/Al and Ni/Ni$_3$Al interface structures was analyzed quantitatively by molecular dynamics (MD) simulations. In particular, the anisotropic diffusion of Al atoms around the interface, which is presumed to be dominant process for the rafting evolution, under uni-axial strain was analyzed.
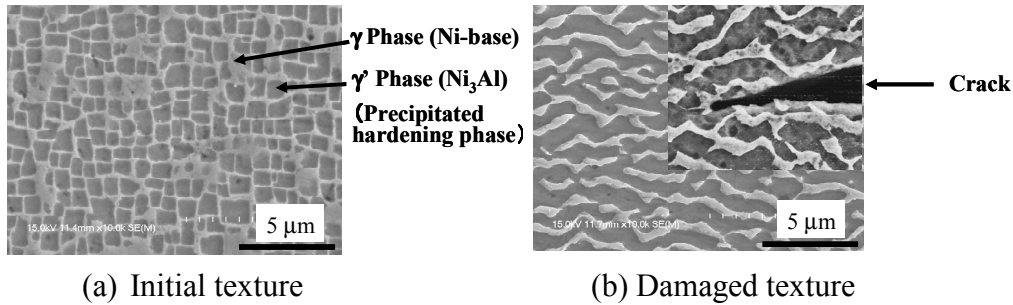
(a) Initial texture   (b) Damaged texture

Figure 1 Micro texture change of Ni-base superalloy caused by creep and fatigue damages

Analytical Model for Molecular Dynamics

In the last decade, computational chemistry has made remarkable progress in the theories and calculation methods and it has a growing role in the field of materials chemistry. It has also been regarded as an efficient tool for obtaining detailed information on atomic scale for diffusion properties. Actually, we successfully simulated the oxygen ion diffusion in strained solid electrolytes [4, 5] and numerous atomistic simulations based on MD have been employed to analyze the characteristics of the interface between γ' and γ phase [6, 7]. In the present study, a simple interface structure between single-crystalline Ni and Al was used as shown in Fig. 2 to analyze the effect of the applied uni-axial strain at the interface with mismatch of lattice constant on the atomic diffusion. Three-dimensional periodic boundary conditions were applied to all calculations. Since Ni and Al are the most important elements in the Ni-base superaloy, this simple analysis shows the idea of the mechanism of the rafting, i.e. the anisotropic diffusion of Al which determines the morphological change of γ' phase in the alloy. The (002) atomic layer corresponds to the coherent interface of Ni(001) and Al(001) in this model. Since large strain more than a few percent exists at the interface due to the lattice mismatch between Ni and Al crystal, the drastic change of the diffusion constant is expected to occur under high strain filed. In addition to the analysis of Ni(001)/Al(001) interface, MD calculations were carried out for Ni(001)/Ni3Al(001) interface to validate the anisotropic diffusion in Ni-base superalloy at elevated temperature of 1173 K. While real γ and γ' phase have other elements such as Co, Cr, etc., we used simple model of pure Ni as γ and Ni_3Al as γ' structure in order to focus the analysis on the anisotropic diffusion of Al in the matrix. To investigate the role of strain on the diffusion characteristics of Ni and Al, we evaluated the self-diffusion coefficient obtained from the slope of mean square displacements (MSD). The interatomic potential defined by Zhou et al [8] was used for the all calculations. This potential is the embedded atom method (EAM) interatomic potential which reproduces the structural features of Ni, Al, and Ni_3Al such as lattice constants, thermal expansion coefficients and so on. Since there is a large mismatch between the lattice constant of Ni and Al crystal, the structural relaxation calculation by changing the volume was performed at 300 K for 10 ps in order to obtain the equilibrium lattice parameters of the Ni(001)/Al(001) supercell model.
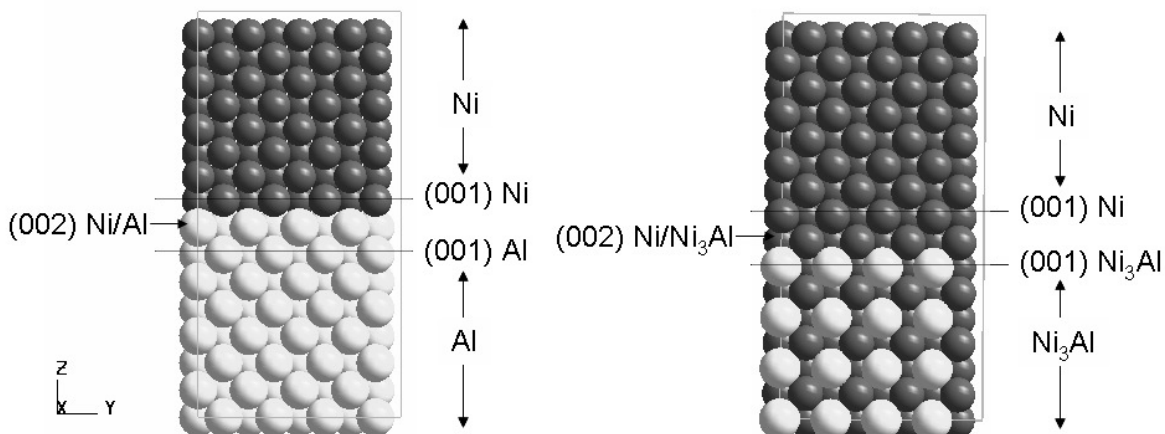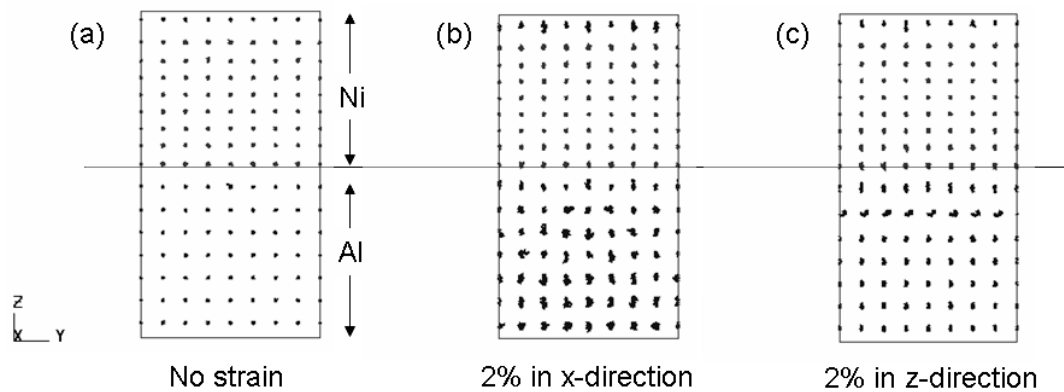
Figure 3 Trajectories of Ni and Al atoms in Ni(001)/Al(001) interface

Results and Discussion

Figure 3 shows trajectories of Ni and Al atoms in the Ni/Al interface structure with (a) 0 % strain, (b) 2 % strain along x-direction (parallel to the interface corresponded to [100] direction) and (c) 2 % strain along z-axis (perpendicular to the interface corresponded to [001] direction). Al atoms diffusion at the interface with tensile strain is increased relative to that in the unstrained interface as shown in Fig. 3. Moreover, this figure also indicates that the mobility of Al atoms at the interface with 2 % strain along x-direction is larger than that with 2 % strain along z-direction. The mean square distance (MSD) of Al perpendicular to the interface (z-direction) increases in both strained interfaces. The strain dependence of atomic diffusion in Ni(111)/Al(111) interface structure was also examined. Slip was found to occur in the both interface structures under strain. It is natural that the slip occurred in the Ni(111)/Al(111) interface under strain because (111) planes in Al crystal are easy to glide to the slip direction (equivalent for x-direction in the interface model) when strain was applied. Since strain caused dislocations and slips in the Ni(111)/Al(111) interface structure, no stress-induced anisotropic diffusion of both Al and Ni at the interface occurred. When stress was applied to the crystal structure, the structure deforms to relieve the applied stress or the high strain energy. However, the slip generation was strictly prohibited in the Ni(001)/Al(001) interface structure because the resolved shear stress within the slip system was not large enough to activate the slip generation. Thus, the anisotropic diffusion perpendicular to the interface occurred to relieve the strain energy. The anisotropic diffusion leads to the mixing of Al and Ni atoms at the interface, resulting in that the lattice mismatch at the Ni/Al interface becomes small and consequently reducing the high strain field. Hence, it is conclude that the stress-induced anisotropic diffusion is expected to occur at the interface for reducing of the strain energy under the elastic condition, which is significantly dependent of the applied load, direction, and interface structure. In order to validate the estimated stress-induced anisotropic diffusion of Al in Ni-base superalloy, MD calculations were applied to the Ni(001)/Ni$_3$Al(001) interface with 2% strain parallel to the interface. Since the Ni/Ni$_3$Al interface has a small strain because of small lattice mismatch between Ni and Ni$_3$Al crystal, the magnitude of diffusion coefficient is smaller than the case of Ni(001)/Al(001) interface. However, it was found that the applied strain enhanced the diffusion of Al atoms perpendicular to the interface (z-direction), which was similar to that observed in the Ni(001)/Al(001) interface system. The diffusion coefficients of Al perpendicular to the interface increases by about 20 times when the uni-axial strain of 2 % is applied parallel to the interface. This diffusion characteristic of Al atoms in Ni$_3$Al phase corresponds the fact that the γ' phase forms layered rafts perpendicular to the stress direction. Therefore, it is highly possible that the morphological change of rafting occurs predominantly by stress-induced anisotropic diffusion of Al atoms.

Since the anisotropic diffusion of Al atoms plays a key role in the rafting phenomenon of γ' phase, the reduction of the mobility of Al atoms perpendicular to the interface between Ni(001) and Ni$_3$Al(001) should decrease the evolution of the rafting and thus, improve both the creep and fatigue resistance of the Ni-base superalloy. The addition of different alloying elements is an effective method for controlling the kinetics of the rafting because it is generally possible to change the lattice
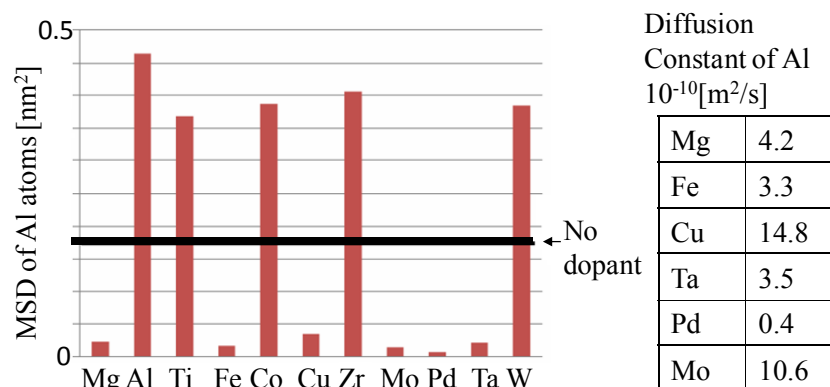
Figure 4 Effect of component elements in Ni$_3$Al on the strain-induced anisotropic diffusion of aluminum atoms

constants of γ and γ' phase, and consequently to modify the coherency stress between the two phases. The effect of component elements in the Ni-base superalloy on the strain-induced anisotropic diffusion of Al atoms was, therefore, analyzed by replacing some Ni atoms in the Ni$_3$Al(001)/Ni(001) interface system by dopant atoms. Tensile strain of about 2% was applied parallel to the interface and the MSD of Al atoms perpendicular to the interface was calculated. Then, the diffusion constant of Al atoms under the strain was calculated by using Einstein's equation. Figure 4 summarizes the effect ofthe dopant element on the MSD of Al atoms under the strain. It was found that Al, Ti, Co, Zr, and W atoms accelerated the strain-induced anisotropic diffusion of Al atoms. On the other hand, Mg, Fe, Cu, Mo, Pd and Ta atoms decreased the diffusion significantly. In particular, Pd is one of the most effective elements which restrain Al atoms from moving around the interface. Both the atomic radius and the binding energy with aluminum of the dopant element are the dominant factors which change the diffusion of Al atoms in the Ni-base superalloy.

Summary

Molecular dynamics (MD) simulation was applied to explicate the strain-induced anisotropic diffusion of component elements of Ni-base superalloy around the Ni(001)/Al (001) and Ni(001)/Ni3Al(001) interface. It was found the diffusion of Al atoms perpendicular to the interface was accelerated by the tensile strain applied parallel to the interface, and thus it should be the main reason for the rafting phenomenon of the micro texture of the superalloy. The dopant elements in the superalloy also affected the strain-induced diffusion of Al atoms. Pd was one of the most effective elements which restrain Al atoms from moving around the interface.

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