

Impurity diffusion in γ -TiAl single crystals

Y. Nosé ^{*,1}, N. Terashita ², T. Ikeda ³, H. Nakajima

The Institute of Scientific and Industrial Research, Osaka University, Ibaraki, Osaka 567-0047, Japan

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Abstract

The diffusion coefficient of In in γ -TiAl single crystals has been measured using the ion implantation technique and secondary ion mass spectrometry in order to clarify the diffusion anisotropy: the diffusion perpendicular and parallel to the [001] axis. The diffusion of In perpendicular to the [001] axis is faster than that parallel to the [001] axis. Such diffusion anisotropy is similar to that of Ti previously investigated by our group. The diffusion coefficients of Fe and Ni have also been measured. The diffusion anisotropies of Fe and Ni show an opposite trend to those of In and Ti, namely the diffusion parallel to the [001] axis is faster than that perpendicular to this axis. The predominant process of diffusion perpendicular to the [001] axis is discussed from the viewpoint of activation energy using the expressions of the diffusion coefficients in $L1_0$ -ordered alloys.

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1. Introduction

The intermetallic compound γ -TiAl has recently attracted much attention as a potential structural material for high-temperature use because of the superior mechanical properties and low density. A knowledge of atomic diffusion is essential to understand such properties from a fundamental viewpoint and in terms of applications.

For γ -TiAl, the tracer diffusion coefficients of ^{44}Ti [1,2] and several substitutional impurity species [3–5] were measured using polycrystalline specimens. Fig. 1 shows the atomic arrangement of γ -TiAl with the $L1_0$ -type ordered structure. (002) planes of Ti and Al atoms alternately stack in the [001] (c -axis) direction. A diffusion anisotropy can be expected from such crystallographic anisotropy. It is

thus necessary to measure the diffusion coefficients in single crystals in order to clarify the anisotropy and the mechanism of atomic diffusion.

Recently, the diffusion coefficients of ^{44}Ti and ^{63}Ni in $\text{Ti}_{47}\text{Al}_{53}$ single crystals have been measured by our group and the diffusion anisotropy has been clarified [6,7]. The diffusion of Ti perpendicular to the [001] axis is faster than that parallel to the [001] axis. The anisotropy of Ni diffusion is less significant. The diffusion coefficient of Fe has been also measured by our group [8]. It has been found that the diffusion of Fe in the direction parallel to the [001] axis is faster than that in the direction perpendicular to the [001] axis. This diffusion anisotropy is opposite to that of Ti. In order to investigate the diffusion mechanism in TiAl, however, it is desirable to measure the diffusion coefficient of Al, which is a constituent element of TiAl.

In the present paper, we report the results of an investigation of the tracer diffusion coefficient of In in TiAl single crystals and its anisotropy. An In tracer is used in this work because of the difficulty of obtaining the radioactive isotope ^{26}Al , which is used for conventional tracer experiments. In is isoelectronic with Al and is expected to show a similar diffusion behavior in TiAl to Al. In fact, Song

* Corresponding author. Tel.: +81 22 215 2013; fax: +81 22 215 2011.

E-mail address: ynose@imr.tohoku.ac.jp (Y. Nosé).

¹ Present address: Institute for Materials Research, Tohoku University, 2-1-1, Katahira, Aoba-ku, Sendai, Miyagi 980-8577, Japan.

² Present address: Toyota Motor Co., Toyota 664-0016, Japan.

³ Present address: California Institute of Technology, 1200 East California Boulevard, Pasadena, CA 91125, USA.

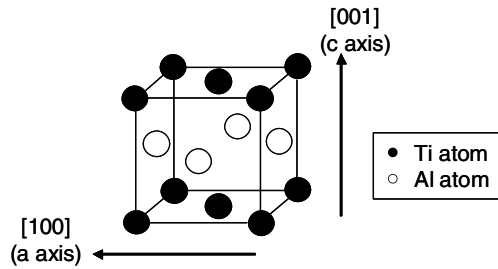


Fig. 1. Atomic arrangement of γ -TiAl.

et al. reported that In atoms preferentially occupy Al sites [9]. The diffusion coefficients of Ni and Fe are also measured in this study and the data are supplemented, since only a few data were available in previous works [7,8]. Furthermore, the diffusion mechanism of these elements in TiAl is discussed using expressions of the diffusion coefficients from the viewpoint of activation energy.

2. Experimental

2.1. Specimen preparation

Ti–54 mol% Al alloy ingots were prepared using an argon arc furnace with appropriate amounts of 99.99% pure Ti and 99.99% pure Al. Single crystals were grown by the floating zone melting method. The bars thus obtained were annealed at 1273 K for 86.4 ks under a dynamic vacuum for homogenization. Two kinds of specimens of $5 \times 5 \times (1-2) \text{ mm}^3$ were cut out from the bars by spark-erosion techniques: the normal vectors of the flat surfaces of specimens were appropriately perpendicular to the [001] axis (specimen I) and parallel to the [001] axis (specimen II). One surface of each specimen was mechanically polished with a series of diamond slurries and finally with $0.5 \mu\text{m}$ diamond slurry on a buff sheet. The orientations of these specimens were determined by the Laue X-ray diffraction method. The deviation of the normal vector of each specimen from the crystal orientation was less than 5° .

2.2. In diffusion by secondary ion mass spectrometry

The compositions of specimens I and II used for the measurement of the diffusion coefficients of In were determined by electron probe microanalysis (EPMA) using a JEOL JXA-8800 in wavelength dispersive mode to be $53.6 \pm 0.2 \text{ mol}\% \text{ Al}$ and $53.2 \pm 0.2 \text{ mol}\% \text{ Al}$, respectively. The intensities of the characteristic Ti $K\alpha$ and Al $K\alpha$ X-rays were measured and converted to compositions using the ZAF method [10]. A $\text{Ti}_{46.8}\text{Al}_{53.2}$ specimen, whose composition had been determined by inductively coupled plasma spectrometry, was used as standard calibration.

For the measurement of the diffusion coefficient of In, the usual experiment method using a radioactive isotope is not adequate since evaporation of the tracer takes place

during diffusion annealing due to the high vapor pressure of In. Therefore, the following process was carried out in this work. The stable isotope ^{115}In was used as a tracer and was deposited onto the surface of each specimen by the ion implantation technique using an NH-20SR-F (Nissin Electric Co. Ltd.) with a Freeman-type ion source. The accelerating voltage was 150 keV, the amount of dosed atoms was $2.0 \times 10^{18} \text{ cm}^{-2}$ and the ion beam was tilted by 5° against the surface of each specimen. The range of ions after the implantation was less than about 80 nm from the surface. Each specimen was wrapped with Ta, Ti and Zr foils to protect from oxidation and sealed in a quartz capsule together with a dummy sample of $\text{Ti}_{42}\text{Al}_{58}$ and pure In of 0.04 g, which were used in order to avoid evaporation of Al and In tracer, respectively, under an argon gas atmosphere after evacuating to better than $2 \times 10^{-4} \text{ Pa}$. Diffusion annealing was done at a temperature in the range 1211–1371 K. The temperature was measured using a Pt/Pt–13% Rh (R-type) thermocouple and controlled to within $\pm 1 \text{ K}$.

After annealing, the penetration profiles were obtained using secondary ion mass spectrometry (SIMS) with a quadrupole mass spectrometer (ATOMIKA SIMS 4100). Ions of O_2^+ , which were accelerated through 10 keV, were used as primary ions. The primary ion beam was tilted by 20° against the surface of each specimen and the scanned area was $300 \times 300 \mu\text{m}^2$. For the analysis, secondary ions from the central area of the crater ($150 \times 150 \mu\text{m}^2$) were extracted to eliminate the effect of the crater edges. The exact depth of each crater was measured after the analysis using a diamond stylus depth profilometer (Dektak IIA, Solan Co. Ltd.). Sputtering rates were determined to be $0.3-0.8 \text{ nm s}^{-1}$. The depth for each sputtering step was then calculated from the sputtering rate and the sputtering time by assuming a constant sputtering rate by the primary ion beam.

2.3. Fe and Ni diffusion by radioactive tracer technique

For the measurements of Fe diffusion coefficients, the compositions of specimens I and II were determined by EPMA to be $53.6 \pm 0.2 \text{ mol}\% \text{ Al}$ and $53.2 \pm 0.2 \text{ mol}\% \text{ Al}$, respectively. For Ni diffusion experiments, the compositions of samples I and II were determined by inductively coupled plasma spectrometry to be $53.2 \pm 1.2 \text{ mol}\% \text{ Al}$ and $53.3 \pm 0.5 \text{ mol}\% \text{ Al}$, respectively.

The radioactive isotopes ^{59}Fe and ^{63}Ni were purchased in the form of an HCl solution from Du Pont/NEN Research Products. The solution of ^{59}Fe was diluted with distilled water and deposited onto the polished surface of specimens by evaporation in a vacuum chamber. For the ^{63}Ni isotope, its solution was diluted to a suitable concentration with dimethyl sulfoxide and distilled water. ^{63}Ni was deposited onto the specimen surface by electroplating using the solution.

The tracer diffusion experiments were done by the same method as previously [6–8]. Specimens together with a

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