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EFFECT OF GRAIN BOUNDARY CHARACTER ON FRACTURE IN COLUMNAR GRAINED Ni_3Al DURING COLD ROLLING*

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Abstract – Polycrystalline Ni_3Al with a columnar grained structure was grown unidirectionally by the floating zone method at a rate of 20 mm/h. Grain boundary structure was characterized by Σ values determined from grain orientations of two adjacent grains using a coincidence lattice theory. Two types of specimens PD and ND, whose cold-rolling directions were parallel and perpendicular to the crystal growth direction, were prepared. Workability and fracture behavior of PD and ND specimens were examined focusing on the effect of the grain boundary character on fracture. PD specimens showed the better workability than ND specimens. Low angle and coincidence boundaries exhibited a strong resistance to grain boundary fracture, while random boundaries were harmful to crack initiation and propagation.

Keywords– Unidirectional solidification, floating zone, texture, coincidence site lattice, coincidence boundary, Σvalue

1. INTRODUCTION

Grain boundary embrittlement in Ni_3Al alloys is a serious problem which should be overcome before industrial application. Many attempts to improve brittle grain boundary fractures have been made by micro- and macro-alloying [1-6]. A small amount of boron addition has been found to be most effective in improving the tensile ductility of Ni_3Al [1, 2].

The ductility of binary Ni_3Al alloys was found to be improved by controlling the grain shape: tensile elongation of cast Ni_3Al alloy containing 24 at %Al increased from 1.2% to 14.1% with a change in grain shape from equiaxed to columnar grains [7]. Stoichiometric Ni_3Al with a columnar grained structure and strong <111> texture, which was unidirectionally grown by using the floating zone method, showed 17% elongation at room temperature without the boron addition [8]. Furthermore, by controlling the crystal growth rate and alloy composition, the columnar grained Ni_3Al alloys exhibited a large tensile elongation of over 70% at room temperature [9] and could be cold rolled to 25% reduction [10]. The nature of the grain boundary is known to be very important for controlling and improving mechanical, chemical and physical properties of polycrystalline materials [11]. Several approaches have been made to improve these properties by controlling the grain boundary character, which is evaluated using Σ values based on the coincidence site lattice (CSL) theory [12, 13].

The CSL can be obtained by allowing the two misoriented crystal lattices adjoining the boundary (crystal I and crystal II) to interpenetrate and translate so that lattice points of each crystal coincide [14]. The space lattice, made up of the coincident lattice is called CSL. The fraction of lattice points in one crystal in good coincidence is defined as 1/Σ. A grain boundary can then be constructed by passing a plane through the interpenetrating crystals and placing all the lattice sites from one crystal on one side of the boundary plane and from the second crystal on the other side of the boundary plane. The reciprocal of the ratio of CSL sites to lattice sites of one of the crystals is denoted by Σ. In general, Σ is large, but for certain boundary

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misorientations it is small [15]. For example, Σ is seen to be 5 for the CSL of Fig.1. The broken lines in Fig.1 denote the (110) planes that terminate at the boundary; they show that the boundary can be considered as a wall of ½(110) edge dislocations. The dislocation spacing is only ¼(130), however, and they bear little resemblance to isolated crystal orientations. The CSL is fundamental to the understanding of the presence of order in high angle grain boundaries. A CSL will occur if each axis of coordinates is simultaneously rotated to become parallel to an original vector [u,v,w] and shares fraction 1/Σ common lattice points with it [16]. Coincident site lattices occur at specific values of 1/θ (axis of misorientation/angle of misorientation), giving rise to a continuous set of structure sites across the boundary. A familiar example of a CSL is the case of a twin in the cubic system. Here a CSL is developed with an overall density of 1 in 3 (written as Σ=3). Depending on the orientation of the boundary plane, the density of common sites may be 1 in 1 on the coherent twin plane and 1 in 3 for an incoherent segment [17].

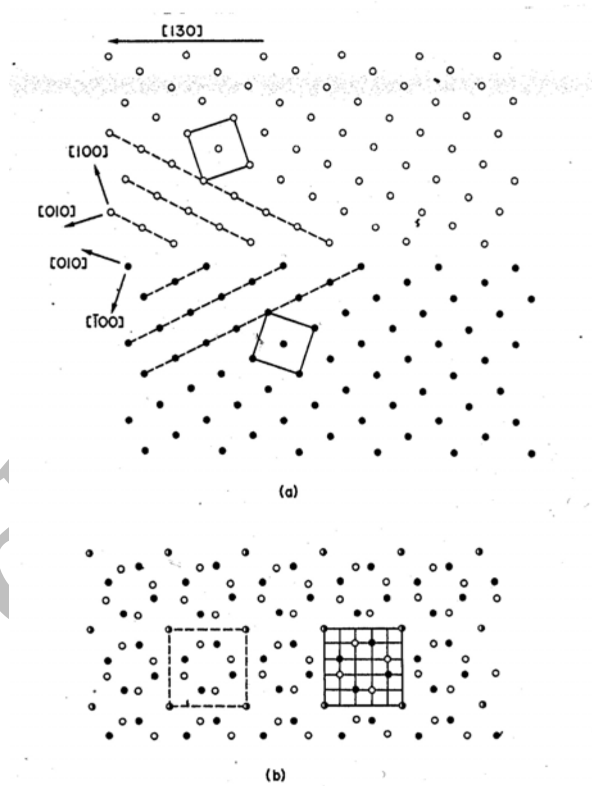

Fig.1. (a) Schematic illustration of the atom positions on a (001) plane in two face-centered cubic crystals separated by a (310) boundary with Σ=5. The unit cells are shown in bold outline. The misorientation angle about [001] is 37° (or alternatively 53°). The projection of atoms on planes immediately above and below the diagram are omitted for clarity. (b) The two lattices of (a) superimposed to show coincident sites, marked as half-filled circles. The unit cell of the CSL is indicated by broken lines on the left, and the DSC lattice is shown on the right [15]

In this paper we describe the effect of the grain boundary character on workability and grain boundary fracture in unidirectionally grown Ni_3Al polycrystals with a columnar grained structure during cold rolling.

2. EXPERIMENTAL PROCEDURE

A master ingot of Ni_3Al with a stoichiometric composition was prepared by arc melting. Polycrystalline Ni_3Al with a columnar grained structure was grown unidirectionally from the ingot by the floating zone method at a rate of 20 mm/h under a high purity argon gas flow. Two types of PD and ND specimens whose rolling planes were chosen to be parallel and perpendicular to the crystal growth direction, respectively, were prepared by spark machining. The rolling directions for PD and ND specimens were chosen to be parallel and perpendicular to the growth direction, respectively. Cold rolling was carried out at room temperature by about 5% reduction for each pass.

Orientation of grains was measured using the scanning electron microscope (SEM)- electron channeling pattern (ECP) technique before cold rolling. Grain boundary structure was characterized by Σ values determined from the SEM-ECPs of two adjacent grains. Brandon's condition was used as the criterion for the exact coincidence orientation relationship [18]. Microstructures and cracks were examined after cold rolling using SEM. Work hardening of cold rolled specimens was monitored by micro Vicker's hardness measurement.

3. RESULTS AND DISCUSSION

In unidirectionally grown Ni_3Al by the floating zone method, a columnar grained structure was obtained in which grains elongated to the crystal growth direction. Figure 2 shows the schematic illustration of grains of a PD specimen before cold rolling. The columnar grains elongate to the crystal growth direction. This specimen was repeatedly cold rolled to the growth direction. Figure 3 shows a schematic illustration of a ND specimen before cold rolling. The bold line shows the Σ1 boundary and the numbers near the grain boundaries represent Σ values of the coincidence boundaries. The shade grains have the normal direction tilted less than 20° from <001>. On the cross section perpendicular to the growth direction, coincidence boundaries and random boundaries are 55.4% and 44.6% of the total number of grain boundaries, respectively. For coincidence boundaries, 42.3% and 3.6% of all the observed boundaries are Σ1 and Σ3 boundaries, respectively. Almost all grains are unidirectionally oriented to <001> direction. Similar strong <001> textured columnar grains in a Ni-24 at %Al-0.2 at %B alloy were produced by directional levitation zone melting [7], while <111> texture was reported in unidirectionally grown Ni-24 at %Al at 24mm/h [8]. Since <001> texture is known to develop in nickel base superalloys during directional solidification, preferential growth parallel to <001> may be a general tendency in Ni_3Al alloy.

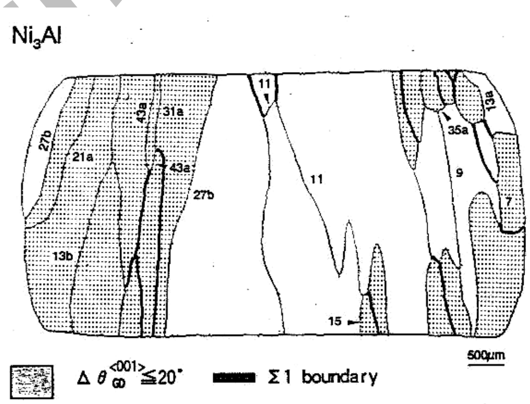

Fig. 2. Schematic illustration of grains and grain boundary character of a PD specimen before cold rolling. The bold boundaries and the numbers represent Σ1 and coincidence boundaries, respectively. The boundaries without the marking represent random boundaries. The shaded grains have their normals tilted less than 20° from <001>

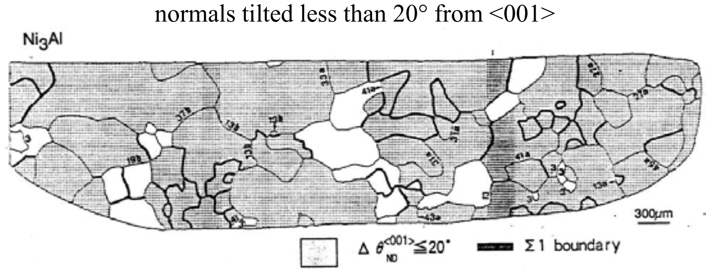

Fig. 3. Schematic illustration of grains of a ND specimen before cold rolling. The marks on the figure have similar meaning to those in Fig. 2

For a PD specimen cold rolled to the growth direction, no severe cracks were observed to a 10% reduction in thickness. As the rolling advances, a crack is initiated and propagates depending on grain boundary character as shown in Fig. 4. Random boundaries seem to be sensitive to cracking by comparison with Fig.2. Although the crack propagation may be heavy depending on grain boundary character, the whole specimen can deform to 42.3% without separating into small blocks. PD specimens show better workability in cold rolling than ND specimens. The columnar grained Ni_3Al was also reported to exhibit a large tensile elongation in the crystal growth direction at room temperature, accompanied by intergranular fracture at peculiar grains [8, 9]. The workability of polycrystalline materials is known to be influenced by such factors as grain orientations, grain boundary character and rolling direction. The effect of grain boundary character in columnar grained Ni_3Al was examined using an ND specimen. As shown in Fig. 5, intergranular cracks are seen in a cold rolled ND specimen depending on grain boundary character. Heavy cracks are observed at random boundaries, while small cracks are formed at Σ1 and Σ3 coincidence boundaries, but further propagation is suppressed.

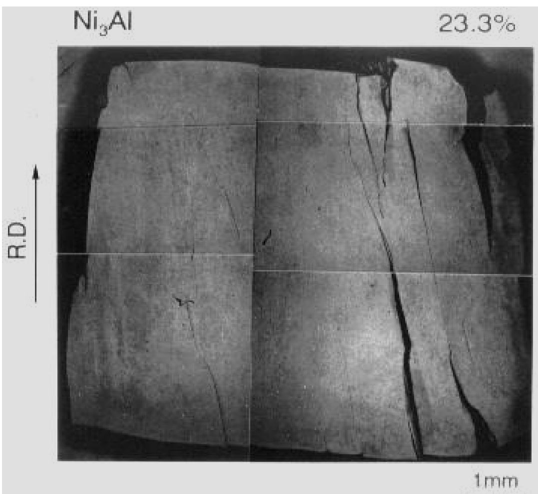

Fig. 4. SEM image of a PD specimen cold rolled to 23.3% reduction

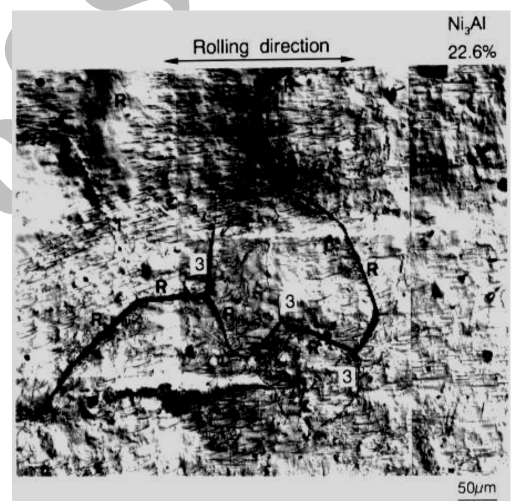

Fig. 5. Cracks and grain boundary character in an ND specimen cold rolled to 22.6% reduction. R and the numbers represent the random boundary and Σ value of coincidence boundary, respectively

Figure 6 shows variation in the number of cracked grain boundaries in measured 222 grain boundaries as the thickness of the specimen is reduced. The data of Figs. 6 and 7 was collected by taking several SEM micrographs similar to that of Fig. 5, and 222 grain boundaries were statistically studied. Random and Σ boundaries were identified, then the samples were cold rolled and cracked boundaries were recorded. At the initial stage of cold rolling, some cracks are observed in a few of the grain boundaries. The frequency of cracked grain boundaries increased with reduction in thickness accompanied by a sharp increase at over 20% reduction. Crack initiation and propagation are known to be very sensitive to grain boundary character. Figure 7 shows change in the frequency of coincidence and random boundaries in cracked grain boundaries. This figure was constructed by detecting the number of cracks and the type of grain boundary in which they occurred. Most cracks occurred in random boundaries at any tested reduction in thickness, while low angle and coincidence boundaries showed good resistance to intergranular fracture. Average micro Vickers hardness in several <001> oriented columnar grains linearly increased from 170 to 500 with cold rolling. A sharp increase in the number of cracked boundaries at above 20% reduction occurred in not only random boundaries, but in coincidence boundaries too. With a reduction of 22.5%, grains were strongly work-hardened, and therefore the residual stress might exceed the strength at the coincidence grain boundary. Frequent crack initiation and propagation at low angle and coincidence boundaries at a reduction of over 22.5% resulted in the fracture of the ND specimen.

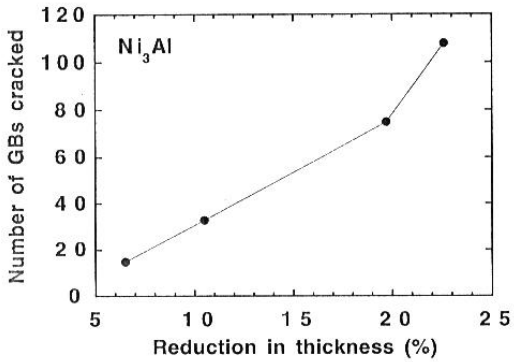

Fig. 6. Variation of the number of cracked grains with the cold rolling reduction in thickness

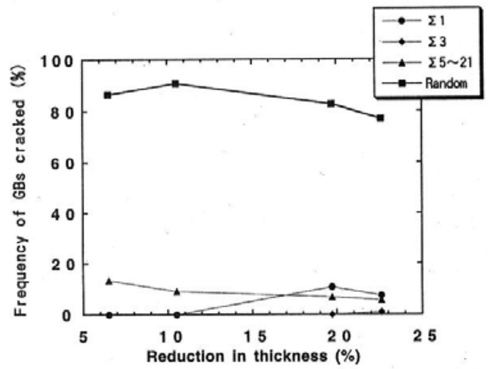

Fig. 7. Change in the frequency of coincidence and random boundaries in cracked grain boundaries as a function of cold-rolling reduction in thickness

Most recently it was found that grain boundaries in Ni_3Al are not intrinsically brittle, but that brittleness is due to an extrinsic factor such as a hydrogen induced environmental effect [6, 19]. The most effective means of suppressing the grain boundary embrittlement is the addition of a small amount of boron, since the diffusion path can be interrupted by a boron dopant. In general, grain boundary diffusion is more enhanced in random boundaries than in low angle and/or coincidence boundaries. In aluminium [20], stainless steel [21] and niobium [22], low angle and some coincidence boundaries were reported to be resistant to corrosion by sulfuric acid. Low angle and some coincidence boundaries with low energy generally show high fracture strength. In Ni_3Al the coincidence boundaries have been found to show less sensitivity to intergranular fractures than random boundaries [23, 24]. The shape and size of grains are known to be important factors for ductility [25]. Although the effect of rolling direction on workability of columnar grained Ni_3Al was observed in the present study, there was no significant evidence of the grain size dependence on grain boundary embrittlement. The most important factor for the intergranular fracture is the grain boundary character and its spatial distribution. The development of microalloying and favorable fabrication processes to obtain high frequencies of low angle and coincidence boundaries with low Σ values are necessary to improve grain boundary embrittlement in Ni_3Al alloys.

4. CONCLUSIONS

The effect of grain boundary character on intergranular fractures in columnar grained Ni_3Al during cold rolling was examined and the following conclusions were reached:

1. A columnar grained structure with a high frequency of low angle and coincidence grain boundaries is obtained in Ni_3Al, unidirectionally grown by the floating zone method. The columnar grained Ni_3Al can be cold rolled to 22.5% and 42.5% reduction in thickness in the rolling directions parallel and perpendicular to the crystal growth direction, respectively, accompanied by the intergranular fracture. The workability depends on the rolling direction; it is more improved in the rolling to the elongated direction of columnar grains.
2. Susceptibility to intergranular fracture depends strongly on the grain boundary character. Coincidence boundaries with low Σ values show good resistance to crack formation, while crack initiation and propagation dominantly occur in random boundaries from an early stage of cold rolling.

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