

GRAIN BOUNDARY DESIGN AND GRAIN BOUNDARY CHARACTER DISTRIBUTION (GBCD) IN TEXTURED POLYCRYSTALLINE MATERIALS

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Abstract

The importance of grain boundary character distribution (GBCD) to materials development by grain boundary design is briefly discussed. Particular attention has been paid to the relationship between GBCD and the nature of texture in polycrystalline materials produced by different processing methods. Several important findings on the relationship are discussed.

1. Grain Boundary Design for Desirable Properties in Polycrystals.

So far it has been well established that the properties of polycrystalline materials are strongly affected by the presence and geometrical configuration of grain boundaries (1). More recently experimental and theoretical studies of the properties and structure of grain boundaries have revealed that the properties of grain boundaries strongly depend on their type and structure (2). Since grain boundaries are potential sites for metallurgical phenomena, the way and the magnitude of the effects of grain boundaries on the bulk properties of polycrystalline materials should be affected by the type and the frequency of grain boundaries, so called 'grain boundary character distribution (GBCD)' (3). The effects of grain boundaries are simply classified into two categories. One is desirable and beneficial effect, and the other is undesirable or detrimental effect. The basic idea of 'grain boundary design' originally proposed by the present author (4) is that if it is possible to suppress the detrimental effect and conversely to increase the beneficial effect, we could endow polycrystalline materials of ordinary composition with much better performance than the original materials. We may regard the grain boundary as a 'material constituent' which has more possibility and versatility dependent on boundary structure than ordinary elements. The possibility and versatility of grain boundaries can be utilized by designing for their best structure, geometry and arrangement in order to improve material performance or to produce a new property. The importance of GBCD to grain boundary design has been recently discussed (5). The presence of a texture is likely associated with a particular GBCD which may be different from that for a random polycrystal.

Therefore, it is of great scientific interest and engineering importance to study the relationship between GBCD and texture in real polycrystalline materials differently produced. The finding of some relationship between GBCD and texture may bring us a clue to the materials development by grain boundary design through texture control.

2. Relationship between GBCD, Texture and Processing Methods.

2-1. Thermo-mechanical Processing: Most engineering metallic material is usually produced by thermo-mechanical processing which consists of plastic deformation and annealing. Many factors associated with plastic deformation and annealing are involved in the processing. When deformed crystal is annealed, recrystallization texture is formed through the generation of new grains and their growth. The nature of the texture in a particular specimen depends on the mechanical and thermal treatments. It is interesting to study GBCD in textured polycrystals which experienced well-defined treatments. It is also important to clarify the factors controlling GBCD and the nature of texture. For these purposes, grain boundaries in polycrystals produced by annealing from deformed single crystals have been studied in aluminium (6-8), molybdenum (9) and nickel (10). However, systematic investigation into GBCD in textured polycrystals has been very scarce (11-13). It has been shown that the frequency of low-angle boundaries, coincidence boundaries and random boundaries depends on the initial

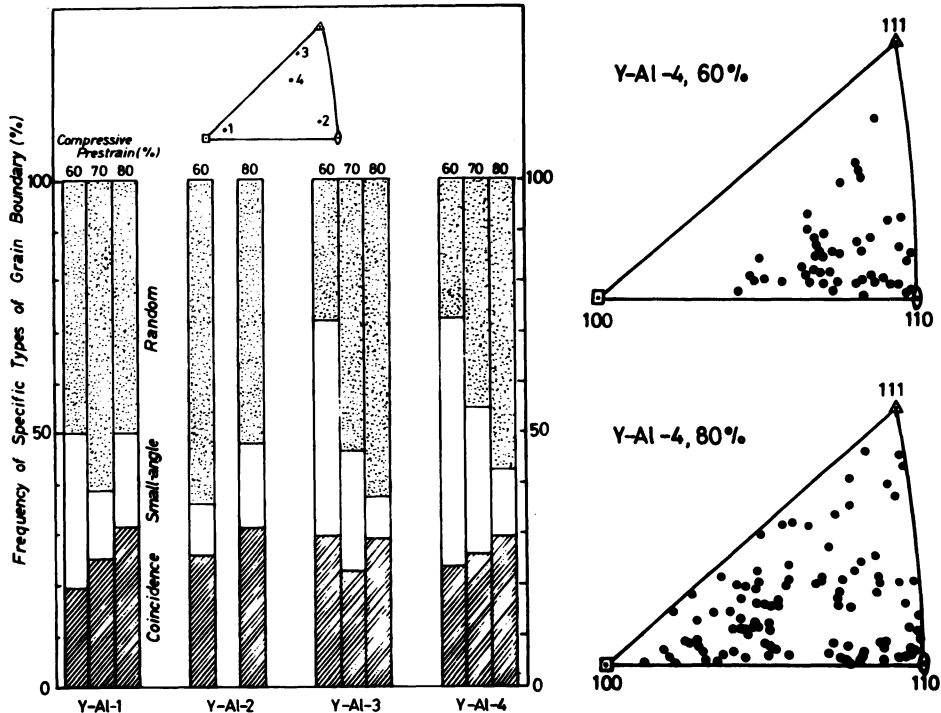


Fig.1 Grain boundary character distribution for aluminium polycrystals produced thermo-mechanically from single crystals with different initial orientations indicated in the triangle.

orientation and the amount of plastic deformation of single crystal, as seen from Fig.1 for aluminium polycrystals (7). The frequency of low-angle boundaries decreased with compressive prestrain. In particular the polycrystal specimens produced from the single crystal sheets with the initial orientations near (112) showed a drastic decrease in the frequency from 42%-49% for 60% prestrain to 8%-13% for 80% prestrain. On the contrary the frequency of random boundaries increased with prestrain. As for the effect of deformation mode, Rybin et al.(9) have found that a molybdenum polycrystal specimen produced by annealing from 85% rolled single crystal contained much higher frequency (65%) of low-angle boundaries than that (11%) for the specimen produced from 83% hydroextruded single crystal. It is surprising that the difference in deformation mode (rolling or hydroextrusion) produces such a large difference in GBCD between the specimens produced annealing under the same condition.

2-2. Rapid Solidification and Annealing: Recently, particular attention has been paid to the metallic or semiconductor materials produced by rapid solidification from the melt. However, until recently little work has been done on grain boundaries in polycrystalline materials produced by this processing and subsequent annealing. The present author and coworkers have studied the GBCD in rapidly solidified and annealed Fe-6.5mass%Si alloy ribbons (12,13). High ductility of the fully annealed ribbons has been ascribed to the presence of a high frequency of low-energy boundaries. As-solidified ribbon had a random grain orientation distribution, but subsequent full annealing at 1369K and 1473K for 1 h produced the (100)- and (110)-texture, respectively. The observed distributions of boundary disorientations are shown in Figs.2(a) and 2(b). It is evident that the distribution is different from that for a random polycrystal indicated by the broken line. Both (100)- and (110)-textured ribbons commonly show higher incidence of low-angle boundaries. Moreover the (110)-textured ribbon shows a bimodal distribution of boundary disorientations and high incidence of high angle boundaries with disorientations around $50^\circ - 60^\circ$. The most important finding associated with GBCD in the textured ribbons is that only those coincidence boundaries which have particular Σ values occurred preferentially as indicated in Fig.3 for the (100)-textured ribbon. The coincidence boundaries with $\Sigma 1, 5, 13$ and 25 occurred preferentially, missing $\Sigma 17$ coincidence boundary which is predicted for the $\langle 100 \rangle$ rotation. In the case of the (110)-textured ribbon, the coincidence boundaries which had the lower Σ values predicted for the $\langle 110 \rangle$ rotation occurred preferentially in descending order of Σ (13). Moreover a new relationship between GBCD and the type of texture has been found which is described by an inverse cubic root Σ law as shown in Fig.4(a). As is clear from the figure, rapid solidification and subsequent full annealing introduced a higher frequency of low-energy low Σ coincidence boundaries. Therefore, it has become possible to predict GBCD in particularly textured polycrystals. This may bring us a clue to predict the grain boundary-

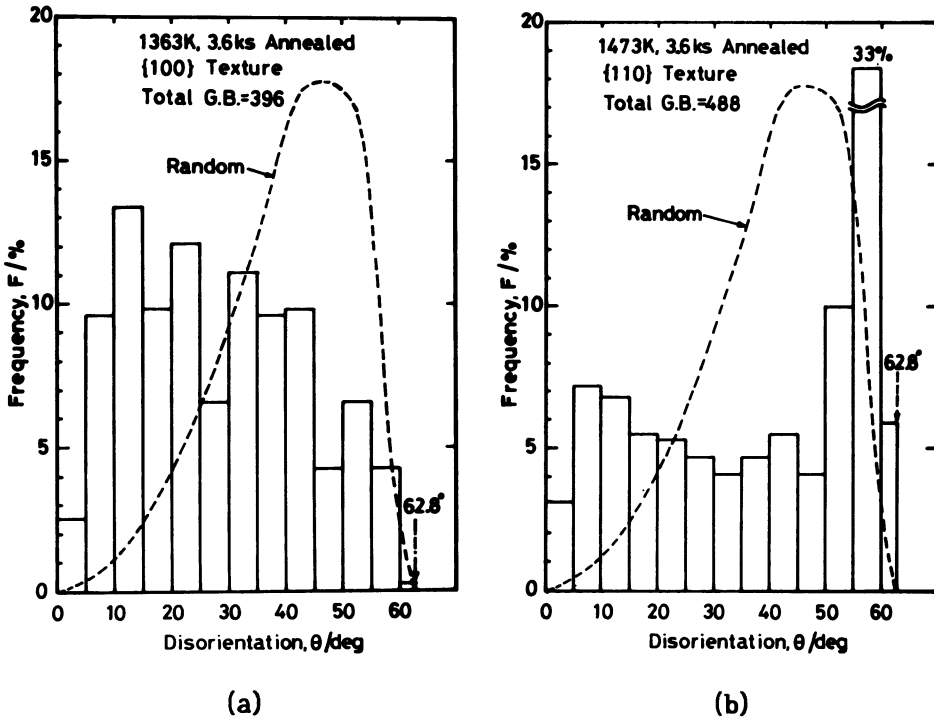


Fig.2(a) and 2(b). Grain boundary disorientation distributions in rapidly solidified and annealed Fe-6.5mass%Si alloy ribbons with (100)-texture (a) and (110)-texture (b).

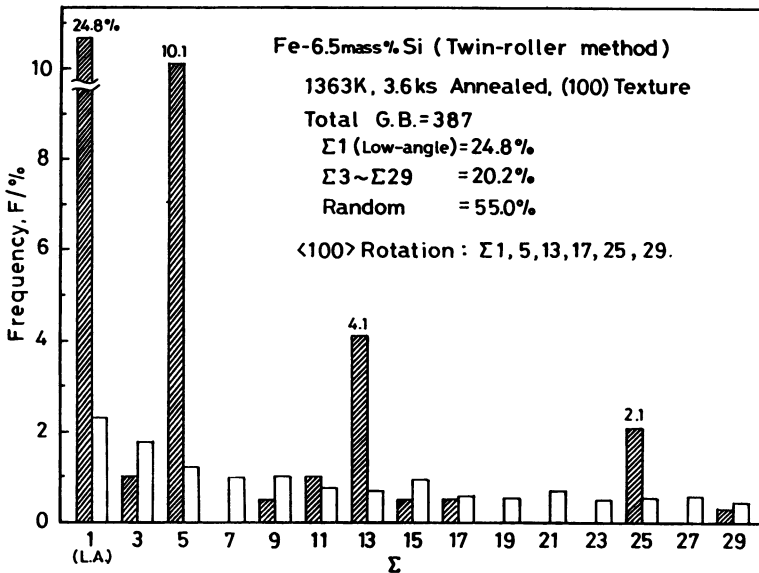


Fig.3 The frequency of coincidence boundaries as a function of Σ in rapidly solidified and annealed Fe-6.5mass%Si ribbon with (100)-texture.

related bulk properties of polycrystals and furthermore to design and manipulate the properties through well-established texture control.

2-3. Unidirectional Solidification: In order to understand special properties of columnar-grained polycrystals produced by unidirectional solidification in connection with GBCD, Watanabe et al. have studied GBCD in columnar-grained specimens of Fe-17%Cr-1%Sn alloy cut from a conventionally cast ingot (14). The specimen had a columnar grain structure elongated to the ingot surface and a strong (100) texture. The characterization of grain boundaries revealed that low-angle ($\Sigma 1$), and coincidence boundaries with $\Sigma 5, 13$ and 17 occurred preferentially as predicted for a (100)-textured polycrystal. Figure 4(b) clearly demonstrates that the frequency of the particular coincidence boundaries in the (100)-textured and columnar-grained specimen of the alloy obeys the inverse cubic root Σ law and is much higher than that for a random polycrystal. It is well known that low energy boundaries have special properties such as high resistance to corrosion, segregation, fracture and so on. High corrosion resistance of the columnar-grained and (100)-textured polycrystals of the Fe-17%Cr alloy can be attributed to the presence of high frequency of low energy boundaries.

2-4. Magnetic Annealing: It has been reported that the annealing of ferromagnetic material in a magnetic field promotes the formation of texture (15). Quite recently Watanabe et al. have studied the GBCD in iron-9mol%cobalt alloy polycrystals received magnetic annealing in the

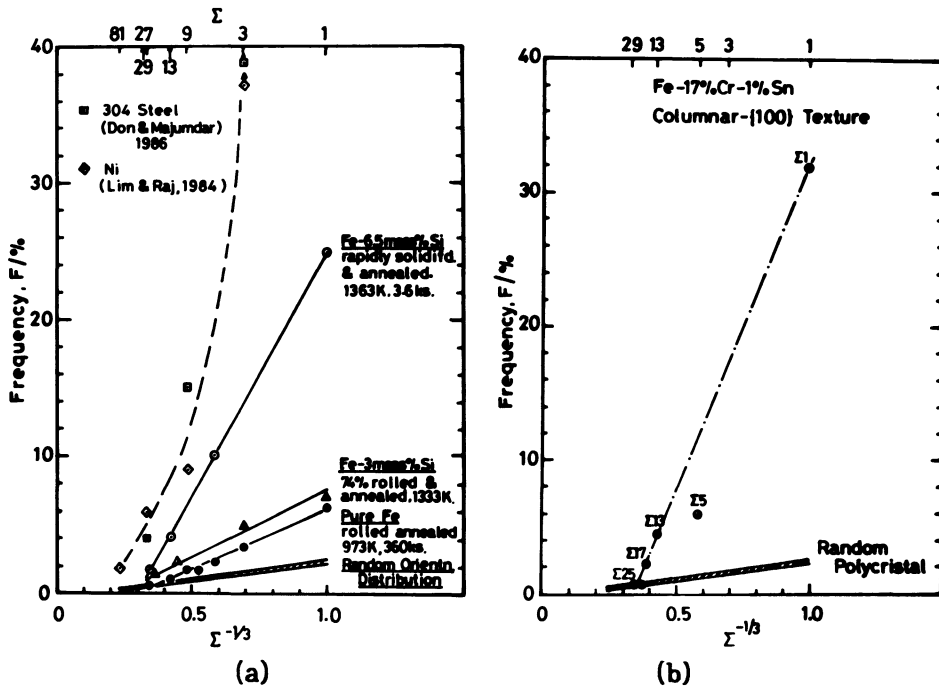


Fig.4. The inverse cubic root Σ dependence of the frequency of coincidence boundaries in differently textured polycrystals of some alloys

field up to 5 kOe (16). It was found that magnetic annealing retards recrystallization and affects the GBCD, particularly the frequency of low angle boundaries in recrystallized polycrystals of the alloy. The frequency of low angle boundaries increases with increasing strength of the magnetic field, exceeding the value predicted for a random polycrystal. This suggests that magnetic annealing can be a powerful tool for controlling GBCD in advanced ferromagnetic or superconducting materials through texture control.

3. The Potential for Grain Boundary Design through Texture Control.

The present paper has discussed the relationship between GBCD and of texture although the state-of-art of this research field is still premature. However the present author believes that the grain boundary design for desirable properties in advanced materials can be achieved by effectively utilizing the knowledge of the relationship between GBCD and texture. Quite recently Garbacz and Grabski have also presented a more detailed discussion on the relationship between GBCD and the type of texture (17). Many unique properties of textured polycrystalline materials should be looked into again from the view point of GBCD.

Acknowledgements

The author deeply thanks coworkers who were involved in the studies relating to the present paper. He also appreciates a Grant-in-Aid for Research from the Ministry of Education, Science and Culture of Japan.

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