Misorientation characteristics of rapid moving boundaries during grain growth in Fe-3%Si alloys

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Abstract. Based on a large amount of experimental observations on highly mobile Σ17, Σ19, and Σ9 coincidence site lattice boundaries (C\text{SLB}), the average jump distances of atoms in connection with misorientation were calculated during boundary migration, which indicated that Σ9 C\text{SLB} demonstrate not only a stable structure, but also higher mobility than other boundaries because of the actual lowest jump distance if the boundaries move. The higher mobility could even keep more or less if the misorientation of boundaries deviates from exact Σ9 in a limited extent. Therefore, Goss grains could grow rapidly in the matrix with many \{111\}<112> grains since the misorientation between Goss and \{111\}<112> is close to Σ9.

1. Introduction
The mobility of grain boundaries in Fe-3% Si alloys has long been a topic of concern and is important in clarifying the mechanism of Goss texture formation in grain-oriented electrical steels. It has been observed that both of the activation enthalpy and the corresponding pre-exponential factor for grain boundary migration in polycrystalline Fe-3%Si alloys are much lower than those observed in bicrystals [1], and the activation enthalpy should be also related with the atom jump distances during boundary migration. Ibe and Lücke conducted the first systematic investigation on boundary mobility in Fe-3% Si alloys, while growth competition of recrystallization grains was observed statistically [2]. The orientation relationship between the crystal matrix and the recrystallization grains that had survived growth competition was determined. The orientation relationships were characterized mainly around 26.7º<110> and 84º<110>, which are very close to the coincidence site lattices (CSL) Σ19 (26.5º<110>) and Σ17 (86.6º<110>), respectively [2], i.e., the corresponding Σ19 and Σ17 boundaries are more active than other boundaries. At the time the study was conducted, however, the reasons behind the phenomena observed were unclear.

Studies have confirmed that Σ9 boundaries in Fe-3% Si alloys are very mobile [3,4]. Goss grains bounded by high frequency Σ9 boundaries [2,5] have been found to grow abnormally with the help of inhibitor particles during secondary recrystallization. High-angle Σ9 boundaries are believed to have lower energies and are consequently less pinned by second phase particles, which induce their higher mobility [4,6]. High frequencies of Σ1 and Σ3 boundaries have been observed in Fe-3% Si alloys, and both boundaries are considered to have significantly low mobility, since Σ1 has low angle misorientation and Σ3 has a twin orientation [3,5]. High frequencies of Σ11 and Σ5 boundaries have also been observed around the periphery of recrystallized grains in Fe-3% Si alloys [3,5]. Given that Σ11 and Σ5 are high-angle and low-energy boundaries, why these boundaries (i.e., Σ11 and Σ5) are not as mobile as that of Σ9 [3] is not yet fully clear.
2. Atom jumps during boundary motion

Grain boundary migration during annealing is a thermal activation process where atoms of one grain jump over the boundary to the atom positions in the lattice of a neighboring grain. The process is rather complicated, and the jump distance plays an important role in the velocity of boundary migration. The activation energy of atomic jumps increases with increasing jump distance. A simplified impression of boundary mobility could be obtained if jump distance, which is related to the difficulty of the atom jump and the magnitude of the corresponding boundary mobility, is calculated and analyzed in a purely geometrical point of view.

Supposing that atoms of a grain rotate around the normal direction [hkl] of an (hkl) plane about an angle and reach the atom positions in the lattice of a neighboring grain, the atoms can jump for different distances on the common (hkl) plane of the two grains regularly when the boundary is in between moves. If the two grains have a common {110} plane, such as in bcc metals, or a common {111} plane, as in fcc metals, the jump distance should be, in general, much lower that those with other common {hkl} planes different from {110} or {111}, since these two planes are the most closely packed planes in bcc or fcc metals. Therefore, the most mobile boundaries often concern a common {111} or <111> in fcc metals [7,8], as well as a common {110} or <110> in bcc metals [2]. The atomic jump distance becomes generally larger than that on a common {110} plane if the atoms jump on another {hkl} plane or if the two grains do not have a common {110} plane, in which case high boundary mobility is not very favorable. Thus, a focused discussion on the misorientation relationships of <110> rotations is necessary when highly mobile boundaries in bcc metals are a concern.

If a (110) plane rotates around its normal direction [110] about a small angle (Fig. 1a), the removed atoms (open symbols) should jump for different distances to reach their original positions (gray symbols). If the plane rotates about such an angle that a CSL is formed between the rotated and original lattices (e.g., Σ9 in Fig. 1b), the atoms at the lattice points of CSL (black symbols) do not need to move in order to recover the original lattice. Figure 1c shows a Σ9 CSL boundary, in which the possible jumps between dashed circles in gray and white are indicated as the CSL boundary between two grains moves.

The average jump distance \( \bar{d} \) of \( n \) atoms can be calculated according to the individual jump distance \( d_k \), in which the two possible atomic arrangements, i.e., the stacking sequence ...ABABAB... of (110) planes, should be considered.

The average jump distance of a (110) plane with about 8 million atoms (2000 × 2000 × 2) was calculated at different rotation angles ranging from 0° to 90°. The average distance, in general, is about 0.369b (in Fig. 2a, b is the length of Burgers vector) for the [110] rotation, except for some special misorientations with low Σ values.
Figure 2. Calculated average jump distances and some Σ values (a) in comparison with the observed frequency of rapid moving boundaries under <110> rotation relations [2] (b). The calculation implies that the lowest average jump distance is 0.215b at 70.53°<110> (Fig. 2a). The corresponding boundary under this misorientation is Σ3; however, the mobility of the boundary in Fe-3% Si alloys is very low because it has a twin orientation [3,5]. The second lowest average jump distance is about 0.3497b at 38.94°<110> (Fig. 2a). The corresponding boundary under misorientation Σ9 is very mobile in Fe-3% Si alloys and can migrate easily as previously reported [3–6]. The average jump distance at many positions with low Σ values is much lower than the general value, which may allow the higher mobility of corresponding CSL boundaries. On the other hand, the average jump distance at some low Σ positions, e.g., Σ11, is higher than the general value, indicating that not all CSL boundaries can offer higher mobility.

3. Discussion

The misorientation of <110> rotations leads to relatively lower average jump distances and higher mobility of corresponding CSL boundaries. Thus, the misorientations of <100>, <111>, or other <uvw> rotations are not discussed firstly. Table 1 shows possible reciprocal densities (Σ≤19) of some CSLs of cubic metals, as well as their corresponding rotation axes and angles. The table shows that Σ5, Σ7, and Σ13 are not described by the misorientation of <110> rotations. As such, Σ5, Σ7, and Σ13 boundaries in bcc metals should not be as mobile as Σ9 boundary. Σ3 represents a twin orientation [3,5] and Σ11 shows a very high average jump distance (Fig. 2a). The only mobile boundaries left at Σ≤19 are Σ9, Σ17b, and Σ19a [9] (Table 1), of which Σ9 may be expected to be the most mobile because it has the lowest average jump distance. The calculations (Fig. 2a), comparison (Table 1), and analysis above agree with observations from Fe-3% Si single crystal experiments for Σ17 and Σ19 boundaries [2], as well as those of Fe-3%Si polycrystalline alloys for Σ9 boundaries [3–6].

Table 1. Possible rotation axis, angles, and reciprocal density Σ of CSL in cubic metals

| Rotation axis | Reciprocal density Σ |
|---------------|----------------------|
| <100>         | 36.87°               |
|               | 22.62°(a)            |
| <110>         | 70.53°               |
|               | 38.94°               |
|               | 50.48°               |
|               | 86.63°(b)            |
|               | 26.53°(a)            |
| <111>         | 60.00°               |
|               | 38.21°               |
|               | 27.80°(b)            |
|               | 46.83°(b)            |

Figure 2b summarizes the misorientation distributions of rapidly moving boundaries in Fe-3% Si alloys, as observed by Ibe and Lücke [2], in which the misorientation distribution around 26.7°<110> also includes the areas of Σ33a, Σ27, Σ9, and other CSL boundaries with low average jump distances aside from Σ19 boundaries (Fig. 2b versus Fig. 2a). Therefore, other CSL boundaries aside from Σ19 are also responsible for the rapid movement of boundaries observed. The atom jumps between two grains without common {110} should not occur on single common plane if a boundary in between moves, and a quite mobile boundary could
then be obtained if the jump distance is short enough, in which the second fastest $\Sigma_5$ boundary [3] might be the case. The detailed mechanism needs to be investigated. Boundary mobility is misorientation-dependent and determined by the orientations of the growing grains and the matrix in which they grow. The texture of Fe-3% Si alloys plays an important role in boundary mobility. Inducing the nuclei of all kinds of orientations during the annealing of 20% rolled single crystals is not possible [2], and the nuclei do not always achieve the frequency necessary to be surrounded by $\Sigma_9$ boundaries. Therefore, while they should show maximum mobility because they have minimum average jump distances (Fig. 2a), $\Sigma_9$ boundaries do not appear with the highest frequency after the growth competition of recrystallized grains (Fig. 2b) [2]. A rather strong $\{111\}<112>$ texture is often observed in rolled and recrystallized Fe-3% Si alloys sheets. The misorientation between the $\{111\}<112>$ texture and the expected Goss $\{110\}<001>$ texture is about $35^\circ<110>$, which is very close to $38.94^\circ<110>$ (Table 1). This observation indicates that Goss grains are commonly bounded by high-frequency $\Sigma_9$ boundaries [2,5], and that the high mobility of $\Sigma_9$ boundaries [3,4] promotes the abnormal growth of Goss grains.

In fact, exact $\Sigma_9$ boundaries are hardly obtained in real Fe-3% Si alloys. The reciprocal density of the CSL becomes extremely large and the jump distance approaches the general value 0.369b (Fig. 2a) by very small deviation from the ideal $\Sigma_9$ boundary (Fig. 1b). The quadrangle in Fig. 1b indicates a unit cell in the $\Sigma_9$ CSL. Similar unit cells can be found when the misorientation is very close to $38.94^\circ<110>$, e.g., at $35^\circ<110>$ (Fig.1d), which indicates that a misorientation occurs between $\{111\}<112>$ and $\{110\}<001>$. The ideal $\Sigma_9$ CSL (Fig. 1b) is more likely to appear with higher stability than with random arrangements (Fig. 1d) if the misorientation of two neighboring grains is very close to $38.94^\circ<110>$. The tendency to form a $\Sigma_5$ CSL in the boundary area of an unideal $\Sigma_9$ CSL (Fig. 1d) increases as the boundary moves closer, and the atomic arrangement tends to change into ideal $\Sigma_9$ CSL cells with some lattice defects. The boundary can then move over rapidly while the average atomic jump distance is shortened, which could explain the high mobility of $35^\circ<110>$ boundaries [3,4].

4. Conclusion
Boundaries between two grains in Fe-3% Si alloys migrate generally faster when a common $\{110\}$ plane exists between them, since the distance an atom jumps in the most closely packed plane becomes generally shorter as the boundaries move. The average jump distances calculated indicate that $\Sigma_9$, $\Sigma_{17}$, and $\Sigma_{19}$ boundaries ($\Sigma \leq 19$) are highly mobile, of which $\Sigma_9$ should be the most mobile. The observed phenomena agree with experimental observations and helps explain Goss texture formation if a certain deviation from $\Sigma_9$ is considered. The mechanism of high mobile $\Sigma_5$ boundary needs to be investigated in this aspect.

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