Influence of grain boundary inclination on the grain boundary and triple junction motion in Zn

Der Einfluss der Korngrenzenorientierung auf Beweglichkeit der Korngrenzen und deren Knotenlinien in Zink

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The experimental results of an investigation of the steady-state motion of individual grain boundaries (GBs) of natural deformation twin and individual twin GBs in bicrystals and tricrystals with triple junction (TJ) are obtained. For experimental observation of GB mobility from the dependence on GB inclination the Zn specimens with individual GBs and TJs were produced. The mobility of natural deformation twin GBs and twin GBs in bicrystals and tricrystals are compared in connection with the GB inclination.

Keywords: Grain Boundary; Triple Junction; Grain boundary Inclination; Coherent twin; Incoherent twin

Die experimentelle Ergebnisse über stationäre Bewegung der individuellen Korngrenzen (KG) wurden gewonnen, und zwar für die Verformungszwillinge und individuellen Zwillingskorngrenzen in Zwei- und Dreikristallen mit Drei-KG-Knotenlinien (TJ). Die Zn-Proben mit individuellen KG und TJ wurden für die Messungen der KG-Beweglichkeit gezogen. Der Einfluss von KG-Orientierung auf Beweglichkeit der natürlichen Verformungszwillinge und gezogenen Zwillingskorngrenzen wurde untersucht.

Schlagworte: Korngrenzen (KG), Drei-KG-Knotenlinien, KG-Orientierung, Kohärente Zwillingsgrenzen, Inkohärente Zwillingsgrenzen

1 Introduction

It is known that the presence of special grain boundaries (GBs) in a material is desirable since the material as a whole would perform better in service [1]. GBs with markedly different properties than those of average GBs are known as 'special'. For many years the coincidence site lattice (CSL) model, which describes GBs in terms of the misorientation between neighboring grains, has been a cornerstone of GB research [2]. It was originally thought that any CSL GB with a low Σ value (where Σ is the reciprocal density of coinciding sites) had special properties. However Wolf indicated that a low-Σ CSL was a necessary but not sufficient criterion for specialness [3]. For instance the so-called "coherent twin" in fcc lattice is a $\Sigma 3$ GB in {111} planes of both grains always possesses special properties whereas the so-called "incoherent twin" which is a $\Sigma 3$ GB lying in a {211} plane may be characterized by "less special" behavior.

GBs can be classified using CSL which defines the periodicity, i.e. the degree of 'fit' between the two lattices which constitute GB. CSLs provide information on particular misorientation between two neighboring grains. Misorientation defines only three of the five degrees of freedom needed to describe GB structure. The other two degrees of freedom are obtained from GB plane orientation.

The importance of knowing GB plane indexes in addition to the misorentation are emphasizes by several researches [4-6]. We observed twin GBs in Zn with the same "matrix/twin" correlation and different space orientation demonstrating dissimilar rate of motion (*Fig. 1*).

The boundary plane geometry can be studied with the aid of bicrystals and tricrystals where all five degrees of freedom are predetermined. The use of fabricated bicrystals and tricrystals allows producing GB with specific plane configuration. Techniques for preparing bicrystals and tricystals are described in [7]. The main reason for using bicrystals and tricrystals is a possibility to measure mobility associated with precisely known GB geometries. In general, GB mobility depends both on GB misorientation and inclination. GB mobility is strongly depends on misorientation [8, 9]. An experimental study the mobility dependence on inclination of GB and TJ with fixed misorientation allows us to understand the inclination effect.

2 Experimental

2.1 Twin grain boundaries

Two kinds of twins exist in materials, namely mechanical (deformation) twins and grown (annealing) twins. The annealing twins are the main structural defects of polycrystals with

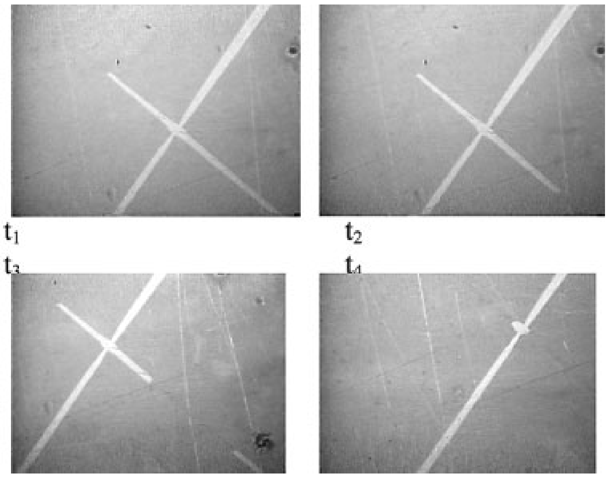

Fig. 1. The line of intersection of the two deformation twins in zinc (99.995 at.%) is perpendicular to the plane of sample. ($t_4 > t_3 > t_2 > t_1$ are annealing times).

Abb. 1. Die Überschneidungslinie zweier Verformungszwillinge in Zink (99,995 at.%) liegt senkrecht zur Probenoberfläeche. ($t_4 > t_3 > t_2 > t_1$ sind Glühungszeiten).

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low and medium stacking fault energy. The deformation twins are the main structural defects of deformed polycrystals. Deformation and grown twins have the same correlation "matrix/twin". We can describe the grown twin GB in terms of axis and angle as GB generated by lattice rotation 86° about axis $[11\bar{2}0]$. Twin GB is special $[11\bar{2}0]$ tilt GB with $\Sigma = 15$.

2.2 Deformation twin grain boundaries

Single crystals were grown by modified Bridgman technique using high purity (99.995 at.%) zinc. By means of an applied stress deformation twins were introduced into the single crystals and we have bicrystal in form of half-loop with two coherent and one incoherent GBs (*Fig. 2* and *Fig. 3*). Coherent GB plane of deformation twin is $(10\bar{1}2)$. Incoherent GB plane as a rule consists of plane lattice facets with low indexes [10]. The using of deformation twins allows one to obtain relatively large driving forces, which is sufficient to force incoherent GB to move.

2.3 Grown twin grain boundaries

Twin GBs in Zn can be presented as the $[11\bar{2}0]$ tilt GBs with lattice rotation angle 86° (See section 2.1). The samples of the bicrystals of Zn (99.999at%) with a twin GB were grown by a modified Bridgman technique in a high purity argon atmosphere in a graphite crucible. Two reversed capillary techniques (*Figs. 4* to *7*), were used to investigate grown twin GB migration: under control variable driving force ("corner" method, Figs. 4 and 5) and under constant driving force ("half-loop" method, Figs. 6 and 7) [8, 11]. In first case the plane of grown twin GBs is under the angle α to basic plane (1000). The major advantages of first technique are the relative ease of manufacturing and preparation of specimen and the possibility to change the driving force by varying angle α to (1000) plane (Fig. 4). This technique allows one to obtain relatively large driving forces under small α. However we can get inclination dependence on GB mobility for low angle interval 0÷20°.

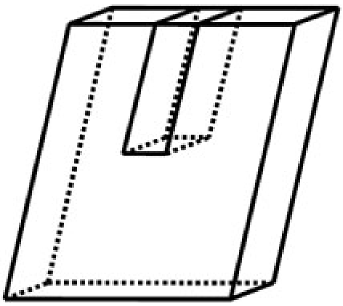

Fig. 2. The scheme of specimen with twin.

Abb. 2. Schema der Probe mit dem Verformungszwilling.

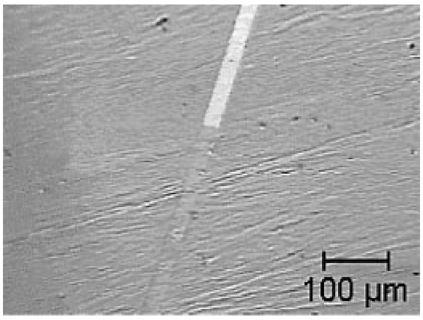

Fig. 3. Micrograph of a twin in zinc (99.995 at.%)

Abb. 3. Lichtmikroskopisches Bild der Verformungszwillinge im Zink (99,995 At.%).

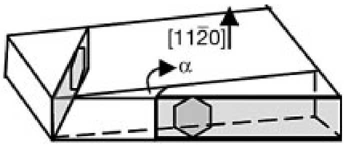

Fig. 4. The scheme for "corner method"

Abb. 4. Schema der „Keilmethode".

The major advantage of a technique with constant driving force is the possibility to change the inclination of grain boundary with the constant angle of misorientation. (Fig. 6). In this case the inclination angle changed between 0÷90°.

2.4 Grown twin grain boundaries with triple junction

The samples of the tricrystals of Zn (99.999 at. %) with TJs were grown by a modified Bridgman technique from single crystalline seeds in high purity argon atmosphere in a graphite crucible, *Figure 8*. In *Fig. 9* the shape of moving GB system

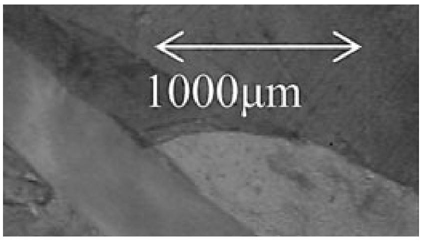

Fig. 5. Individual video frame of GB migration.

Abb. 5. Bild aus der Videoaufnahme der KG-Bewegung.

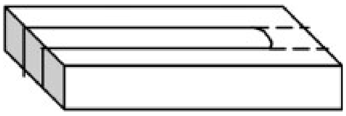

Fig. 6. The scheme for "half loop method".

Abb. 6. Schema der „Halbschlingemethode".

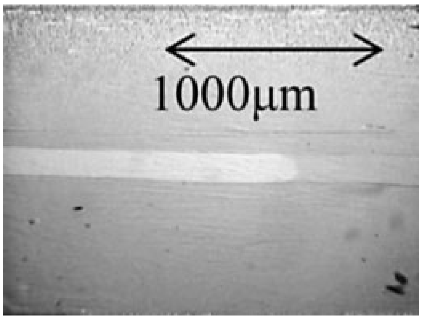

Fig. 7. Individual video frame of GB migration.

Abb. 7. Bild aus der Videoaufnahme der KG-Bewegung.

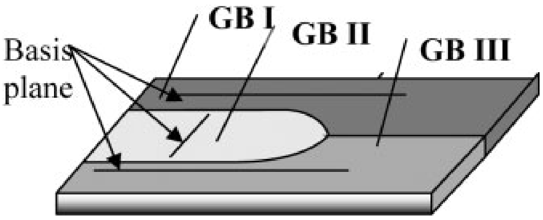

Fig. 8. The geometry of tricrystalline specimen with TJ.

Abb. 8. Geometrie eines Dreikristalls mit der Drei-KG-Knotenlinie (TJ).

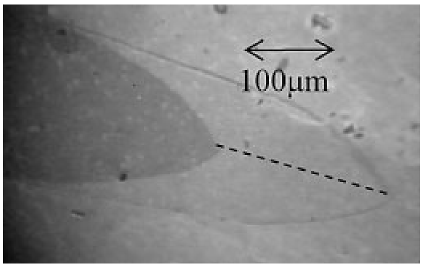

Fig. 9. The shape of two moving GBs and TJ.

Abb. 9. Die Form zweier bewegender KG und TJ.

with TJ is shown. The sample contents two curved high angle tilt GBs, $[11\bar{2}0]$ 84° and $[11\bar{2}0]$ 87°, and a straight 3° tilt GB (not visible in the pictures, it ranges from the tip of the junction parallel to the straight part of the high angle GBs to the low right corner of the pictures).

3 Results and discussion

To study *in-situ* the migration of twin GBs and system of twin GBs with TJ at elevated temperatures a modified optical microscope with polarised light and a hot stage was used. An additional polarisation filter applied in the reflected beam allows distinguishing the different orientations of the grains by the different intensity of the reflected light. By rotating the sample with respect to the incident beam the contrast was enhanced. The experiments were carried out in the temperature range 473 to 683 K. It is possible to determine the mobility of system from time dependence of GB or TJ displacement and a shape of moving GB or TJ at any moment. We consider the steady-state motion of GBs and TJs in the system of grown twin GBs. GBs and TJs in our configurations are straight and perpendicular to the plane of the diagram. Away from TJ all three GBs have to be planar and their planes are parallel to one another and perpendicular the plane of the diagram. This makes the problem quasi-two-dimensional.

The driving force was provided by reduction of the free energy of the boundaries and reads (per unit area):

$$p = \frac{2\sigma}{a}, \tag{1}$$

where σ is the surface tension of GB and a is the width of the shrinking grain. The mobility of GB is given by the ratio of velocity v and driving force p:

$$m = \frac{v}{p} = \frac{va}{2\sigma} \tag{2}$$

In our experiments we used the reduced mobility A [12]:

$$\mathrm{A} \equiv \frac{\mathrm{va}}{2} = \mathrm{m}\sigma = \mathrm{A_0 exp}\left(-\frac{\mathrm{H}}{\mathrm{kT}}\right) \tag{3}$$

where H is the activation enthalpy and A_o is the preexponential factor. The reduced mobility depends on activation enthalpy H and preexponential factor A_o. We suppose the inclination effects on H and A_o is different. We decided to divide the influence the inclination on H and A_o and to investigate the influence the inclination on parameter A_o. *Fig. 10* shows the typical Arrhenius plot of the twin GB mobility. At low temperatures the motion is thermally activated process, at high temperatures the motion is athermal. The effect of the athermal grain boundary motion was observed in our early works in Zn only, the nature of the athermal motion was not clear [13, 14]. The influence of anisotropy is the one of the main reasons of athermal motion of grain boundaries in zinc [15].

Obviously it is best to study the inclination dependence of a boundary where the athermal motion is most marked. It has been found that effect is only observed in special GBs in Zn. We investigated the inclination dependence on the motion of natural deformation and grown twin GBs because twin GB is special. Moreover, we observe that twin GBs with the same "matrix/twin" correlation and different space orientation demonstrate dissimilar rate of motion (Fig. 1).

3.1 Deformation twin grain boundaries motion

Shrinkage of twin proceeds by incoherent twin GB motion along coherent twin GBs during annealing under high temperature. Large velocities of GB motion are obtained in motion under high driving force. Deformation twin GBs exhibit low mobility, it is necessary to create high driving force, i.e. very small dimension of half- loop (Fig. 2.) Athermal GB migration was experimentally observed for deformation twin GBs (*Fig. 11*). The temperature dependence of the mobility is characteristic for breakaway of migrating GB from its adsorbed impurities [16-19]. Essential new features are that before and after detachment from the impurity atmosphere the GB mobility is temperature independent. The motion of individual incoherent twin GB was investigated in the temperature interval between 473 and 681 K.

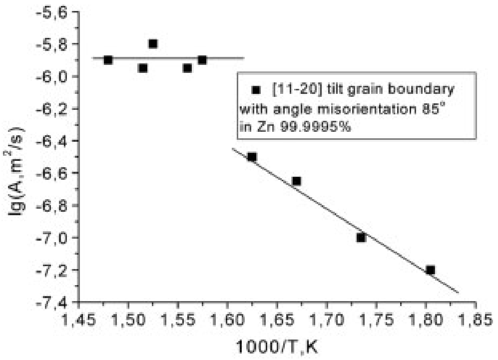

Fig. 10. The temperature dependence of twin GB mobility in zinc bicrystal.

Abb. 10. Die Temperaturabhängigkeit der Beweglichkeit der Zwillings-KG in einem Zn-Bikristall.

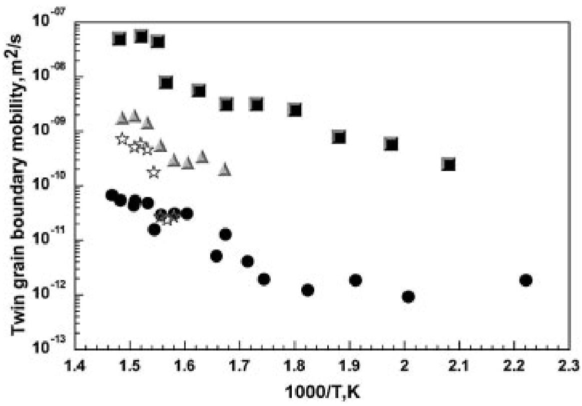

Fig. 11. Temperature dependence of twin GB mobility and twin GB mobility with triple junction, ■ Grown twin GB, ★ Triple junction with grown twin GBs ([11$\bar{2}$0] tilt GBs ϕ_1=82°, ϕ_1=80°,ϕ_1=2°), ▲ Triple junction with grown GBs ([11$\bar{2}$0] tilt GBs ϕ_1=84°, ϕ_1=87°,ϕ_1=3°), ● Deformation twin GB

Abb. 11. Die Temperaturabhängigkeit der Beweglichkeit der Zwillings-KG ohne und mit TJ, ■ Gezogene Zwillings-KG, ★ TJ mit gezogener Zwillings-KGs ([11$\bar{2}$0] Kipp-KG mit ϕ_1=82°, ϕ_1=80°,ϕ_1=2°), ▲ TJ mit gezogener Zwillings-KGs ([11$\bar{2}$0] Kipp-KG mit ϕ_1=84°, ϕ_1=87°,ϕ_1=3°), ● Verformungszwilling.

3.2 Grown twin grain boundaries motion

Fig.10. shows the temperature dependencies of the mobility of [11$\bar{2}$0] tilt GBs, angle misorientation 86°±0.5°. Atermal GB migration was experimentally observed for grown twin GBs (Fig. 10). The temperature dependence of the mobility is characteristic for breakaway of migrating boundary from its adsorbed impurities [16-19]. An essential new feature is that GB mobility is temperature independent after detachment from the impurity atmosphere. The motion of individual grown twin GB was investigated in the temperature interval between 548 K and 681 K. A characteristic feature of the observed dependence is a drastic change of the GB mobility in a narrow temperature range. Below the breakaway region GB mobility demonstrates a usual Arrhenius-type temperature dependence Figs.10 and 11.

3.3 Grown twin grain boundaries motion with triple junction

Fig. 11 shows the temperature dependencies of the TJ mobility. We observe the athermal TJ motion. It is known that the motion of GB systems with TJs in Zn can be controlled by slowly moving TJs and by GBs. The influence of TJs depends on temperature. It is particularly strong at temperatures below $0.85T_m$ in Zn (T_m is a melting temperature). In the temperature interval above $0.85T_m$ the motion of a connected GB system is less affected by TJ, and, therefore, effectively controlled by GB mobility [20, 21]. Contrary to the motion of an individual GB, there is new aspect of the problem where inclination influence can manifest itself, namely GB faceting in TJ, because the whole angle at triple point is 2π. The theories of inclination influence on GB motion also can be applied with certain corrections to TJ motion.

3.4 The influence of inclination on twin grain boundaries motion and twin GBs motion with triple junction

It was found that kinetic parameters of GB depend strongly on GB inclination. There were observed three kinds of twin GB motion: **1.** Activated motion in a wide range of temperatures. **2.** Activation-less motion. **3.** Activated motion at low temperatures combined with activation-less motion at high temperatures. It has been established that the transition from activated to activation-less motion has a jump-wise character. The shape of a boundary will be a smooth curve as long as the boundary surface tension varies continuously. If, however, it changes discontinuously with GB inclination faceting of the moving grain boundary would occur [10, 18]. The scheme of bicrystals with grown twin GB with different orientations of GB plane and dependence of the twin GB mobility in bicrystals vs. inclination angle θ at 673 K are presented on *Figs. 12* and *13*. The angle of inclination θ was found as the angle between basic plane (1000) in one grain and the plane of GB. Fig. 13 shows experimentally determined curve of the GB mobility of tilt [11$\bar{2}$0] GBs with misorienatation angle 86° on athermal intercept as a function of inclination θ (0, 4, 14, 19, 22, 30, 45, 60 and 90°). The angle of inclination θ was imparted in the process of fabricated GB. As we can see, the GB mobility varies non-monotonically with θ and amplitude is quite large

$$\frac{A(\theta = 20^o)}{A(\theta = 90^o)} \cong 10^3$$

The values of natural deformation twin GB mobility and TJ mobility coincide with this curve.

4 Conclusions

Twin GB motion has been observed.

1. The mobility of grown twin GB vs. inclination angle θ, measured by "half-loop method", the mobility varies non - monotonically with θ and amplitude is quite large $\cong 10^3$. The experimental results show the strong effect of the GB inclination on kinetic properties of GBs and

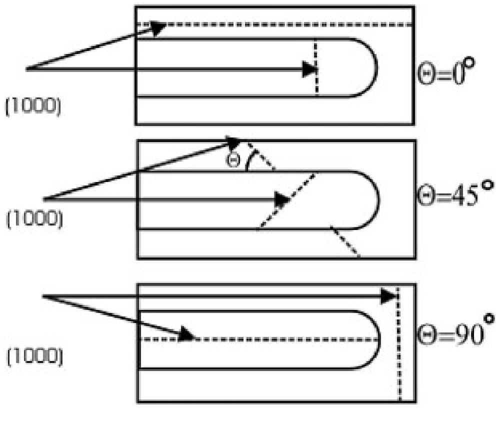

Fig. 12. The scheme of bicrystals with grown twin GBs with different orientations of GB plane

Abb. 12. Schema eines Bikristalls mit gezogenen Zwilling-KG, deren KG-Fläche unterschiedlich orientiert ist.

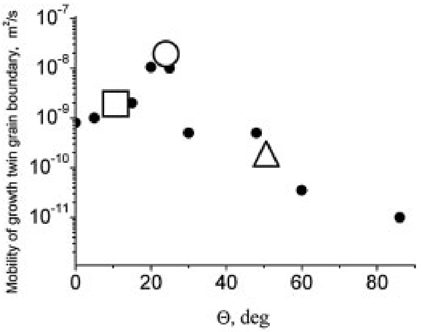

Fig. 13. Dependence of twin GB mobility in bicrystals vs. inclination angle θ at 673 K. Open ring corresponds to the mobility of twin GB in a bicrystal measured by “corner method”. Open square corresponds to the mobility of twin GB in a tricrystal measured from GBTJ experiments. Triangle corresponds to the mobility of deformation twin GB. Filled rings correspond to the mobility of twin GB in bicrystals with different inclination θ measured by a “half-loop”

Abb. 13. Die Abhängigkeit der Beweglichkeit der Zwillings-KG in Bikristallen von dem Orientierungswinkel (Inklinationswinkel) θ bei 673 K. Offener Ring entspricht der Beweglichkeit der Zwillings-KG in einem Bikristall gemessen mit der „Keilmethode. Quadrat entspricht der Beweglichkeit der Zwillings-KG in einem Trikristall gemessen in den Experimenten mit TJ. Das Dreieck entspricht der Beweglichkeit des Verformungszwillings. Offener Ring entspricht der Beweglichkeit der Zwillings-KG in Bikristallen mit unterschiedlichen Inklinationen θ gemessen mit der „Halbschlingemethode“.

TJs in zinc. It may be attributed to GBs structure variation in dependence of the GB inclination.

2. It has been found that the mobility of GBs of deformation twin is 3 orders of magnitude less than the mobility of grown twin GBs (Fig. 11). It clearly demonstrates the role of the GB inclination.
3. The temperature of sudden mobility change which can be interpreted as detachment from an impurity cloud is 573 K for twin GBs obtained by deformation. Deformation twin GBs manifest athermal motion before and after detachment from an impurity cloud. It is supposed that it is the result of low adsorption capacity of differently oriented twin facets.
4. It has been shown previously that the TJ mobility is controlled by GBs at high temperature, and, therefore, TJ does not drag the motion of GBs system with TJ. It is suggested that the adsorption capacity of TJ line is low at temperatures more than $0.85T_m$. Therefore, we may suppose that the observe sudden mobility change during GBs motion with TJ is controlled by the detachment of GBs from impurity cloud, and not by TJ. The additional prove of this conclusion is based on the fact that the mobility changes suddenly at the same temperature of 643 K for grown twin GB both with and without TJ.
5. It has been found that the mobility of grown twin GBs connected by TJ is by 2 orders of magnitude lower than the mobility of single fabricated twin GBs without TJ both before and after detachment (Fig. 11). It is the influence of TJ.
6. The fabricated twin GBs connected by TJ manifest athermal motion at temperatures above sudden mobility increase. If a sudden mobility change is driven by the detachment from impurity cloud, the athermal motion at high temperatures can be explained by the low adsorption capacity of the fabricated twin GBs.

Acknowledgments

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