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Impact of grain boundary character on grain boundary kinetics

Dedicated to Professor Dr. Dr. h. c. Herbert Gleiter on the occasion of his 65th birthday

The current research on grain boundary dynamics in metals is reviewed. The boundary dynamics, i. e., the boundary reaction to applied forces, is strongly dependent on the grain boundary character, which is commonly reduced to the orientation relationship between adjacent grains and impurity segregation at the boundary. The misorientation dependence of the motion of specific capillary driven grain boundaries, the effect of inclination on the mobility of planar boundaries and the dislocation absorption by moving boundaries are considered. The role of segregation behaviour and boundary crystallography for the orientation dependence of boundary mobility is addressed. The compensation effect for the motion of structurally different grain boundaries is discussed.

Keywords: Grain boundary; Misorientation; Inclination; Driving force; Migration; Mobility; Segregation

1. Introduction

Important microstructural changes in metallic materials are introduced by heat treatment subsequent to plastic deformation. By recrystallization and grain growth the defect density and orientation distribution of grains are markedly affected which, in turn, drastically changes the material properties. The fundamental processes of recrystallization and grain growth are the motion of grain boundaries (GBs), by which the crystalline solid is reconstructed atom by atom. Polycrystalline solids possess a wide variety of structurally different boundaries, which quite differently react to exerted forces. In his seminal review [1] Gleiter reported on the effect of grain boundary crystallography on grain boundary properties, like energy and kinetics. GBs have the unique property to move under the action of a driving force, which to a great extent is determined by the grain boundary crystallography as defined by the misorientation between adjacent grains and the orientation of the boundary plane. The role of orientation relationships for GB dynamics will be addressed in this paper.

2. Fundamentals of grain boundary dynamics

2.1. Driving force

A driving force p for GB migration occurs, if the displacement $d\ell$ of a boundary area s leads to a decrease of the total

Gibbs energy dG of the system:

$$p = - \frac{dG}{s \cdot d\ell} = - \frac{dG}{dV} \quad (1)$$

where V is the volume swept by the boundary area during its displacement. The gain of Gibbs energy can result from a change in grain boundary energy due to a reduction of the GB area in case of curved capillary-driven boundaries, or from a volume Gibbs energy difference across the boundary, e. g. by the anisotropy of Gibbs energy density in a magnetic, electric or elastic field.

2.2. Measurements of grain boundary motion

Since there is no average representative grain boundary in a crystalline solid, GB properties are most appropriately measured on specific individual GBs, i. e., in specially prepared bicrystals. Equivalently, the measurement of connected GB systems with junctions requires tricrystal experiments, etc.

There are two different ways to determine the GB velocity. In the discontinuous method the location of the boundary is determined at discrete time intervals by the position of a boundary groove. The advantage of this stepwise annealing method is its simplicity, but its main shortcoming is that the measured boundary velocity is averaged over the large interval of time between consecutive observations. In contrast, the continuous method requires to determine the boundary position at any moment of time without forcing the boundary to stop. This is achieved by utilizing orientation dependent properties and their discontinuity at the GB. There are various techniques to distinguish different crystal orientations. Most measurements so far were conducted with the X-ray interface continuous tracking device [2]. The method employs X-ray diffraction to determine the GB position and, therefore, does not interfere with the boundary migration process itself. The device can measure a boundary velocity in a wide range between 1 and 1000 $\mu\text{m/s}$. Its inaccuracy amounts to less than 2% [2]. For time-resolved imaging of connected GB systems (junctions, networks) the orientation dependence of backscattered electrons in a scanning electron microscope can be used [3]. In materials with noncubic crystal symmetry, the anisotropy of reflectivity of visible light can be utilized for the orientation contrast to determine the boundary location.

2.3. Grain boundary mobility

GB motion consists of the transfer of lattice sites across the GB, which results in a physical displacement of the GB with regard to an external reference frame. Atoms crossing the boundary will change their energy state (Fig. 1) which results in an asymmetry of the atomic migration energy and thus an imbalance of the jump rate across the boundary in opposite directions.

Each atom of volume $\Omega_a \approx b^3$ will gain the Gibbs energy pb^3 when becoming attached to the growing grain but has to expend this Gibbs energy when moving in the opposite direction. Correspondingly, with a boundary displacement b per atom the boundary velocity reads

$$v = bv_D \left(e^{-\frac{G_m}{kT}} - e^{-\frac{G_m+pb^3}{kT}} \right) \quad (2)$$

(v_D – Debye-frequency, G_m – activation Gibbs energy of boundary migration, k – Boltzmann’s constant, T – absolute temperature).

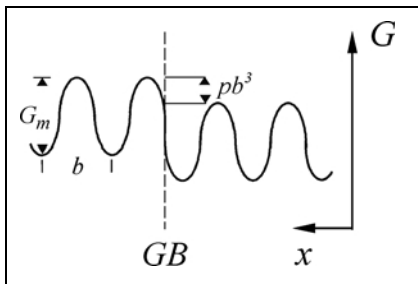


Fig. 1. The Gibbs energy of a moving atom changes by the driving force pb^3 when it crosses the boundary. G_m is the Gibbs energy barrier for atom transfer.

For all practical cases $pb^3 \ll kT$ at temperatures where boundaries are observed to move ($T \geq 0.3T_m$) and, therefore,

$$v = \frac{b^4 v_D}{kT} e^{-\frac{G_m}{kT}} \cdot p \equiv m \cdot p \quad (3)$$

The quantity m is referred to as grain boundary mobility.

GB migration is a thermally activated process. Thus, its kinetics follow an Arrhenius-type temperature dependence

$$v = v_0 \exp\left(-\frac{H}{kT}\right) \quad (4)$$

Since the driving force is essentially independent of temperature, the temperature dependence of v is the temperature dependence of the grain boundary mobility

$$m = v/p = m_0 \exp\left(-\frac{H}{kT}\right) \quad (5)$$

where H is the activation enthalpy of GB migration and m_0 the corresponding pre-exponential mobility factor.

For the migration of curved GBs, we introduce for simplicity the reduced mobility

$$A = m \cdot \sigma_b = A_0 \exp\left(-\frac{H}{kT}\right) \quad (6)$$

where σ_b is the grain boundary surface tension.

Since the reduced mobility is the product of mobility and GB energy, it reflects also the orientation and temperature dependence of the GB energy. However, according to com-

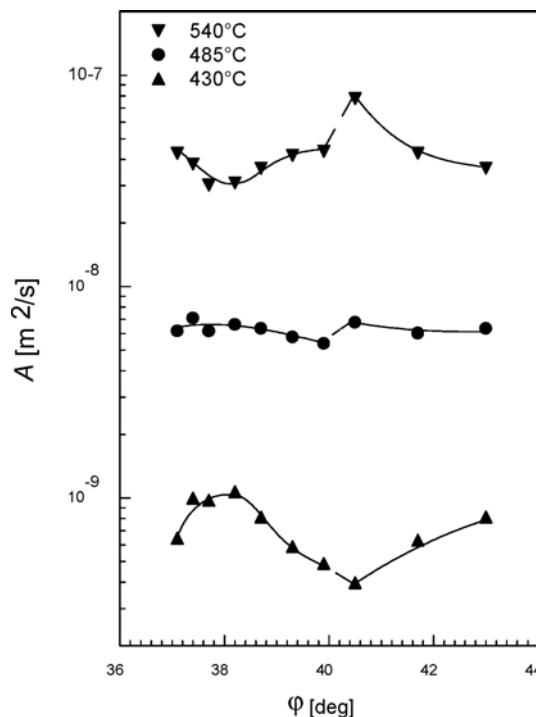
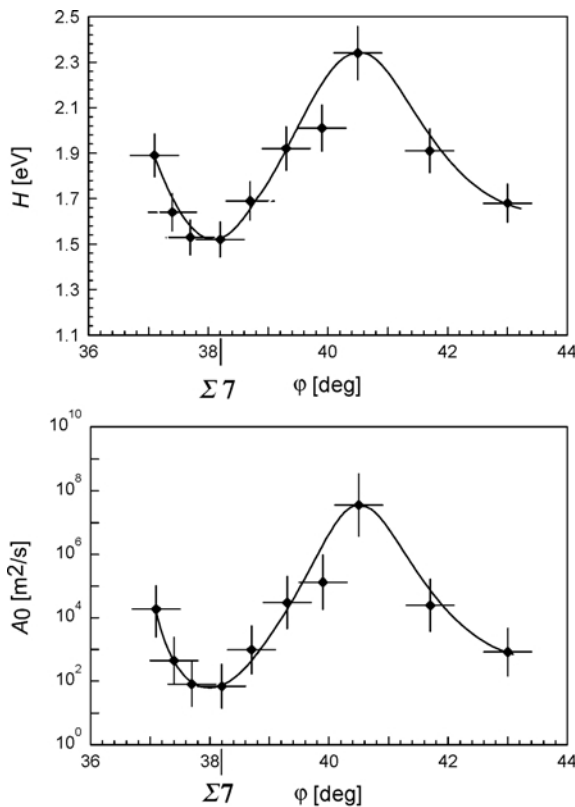


Fig. 2. (a) Activation enthalpy H and pre-exponential factor A_0 for $\langle 111 \rangle$ tilt GBs and (b) mobility dependence of $\langle 111 \rangle$ tilt boundaries on rotation angle in pure Al (99.999%).

puter simulations and measurements, the GB energy may change by 20 % or less but the reduced mobility will change by orders of magnitude. Therefore, changes of the GB energy can be neglected, if not absolute mobility values but activation parameters and mechanisms of GB motion are considered, as in the case of investigations referred to in the following.

3. Misorientation dependence of grain boundary mobility

3.1. Misorientation of adjacent grains

It was already shown in the past in bicrystal experiments of Rutter and Aust [4] and Shvindlerman with coworkers [5–7] that for high-angle GBs the mobility depends on axis $\langle hkl \rangle$ and angle φ of misorientation. Studies of the mobility of tilt GBs in Al bicrystals [5] have shown that the mobility of low Σ coincidence boundaries (special boundaries) exceeds the mobility of random (nonspecial) boundaries. Among all tilt boundaries those with $\langle 111 \rangle$ rotation axis and rotation angle of about 40° were found to have the highest mobility, which is associated with the special $\Sigma 7$ tilt boundary.

However, from growth selection experiment [8–10] it was known that the rotation angle of the fastest boundaries was invariably larger than 38.2° even consistently larger than 40° .

Owing to the importance of maximum growth rate boundaries for texture formation during recrystallization and grain growth we addressed this obvious discrepancy, and investigated the misorientation dependence of GB mobility on a fine scale in the angular interval 37° – 43° $\langle 111 \rangle$ with angular spacing 0.3° – 0.6° [11, 12]. The experiments revealed that both the activation enthalpy and the pre-exponential factor were at maximum for a misorientation angle $\varphi = 40.5^\circ$ and at minimum for the exact $\Sigma 7$ misorientation (Fig. 2). Therefore, one is tempted to conclude that the $\Sigma 7$ boundary has the highest mobility. However, the mobility of boundaries with different misorientation an-

gles do have a different temperature dependence, and there is a temperature, the so-called compensation temperature T_c , where the mobilities of all investigated boundaries with different misorientation are the same. As a result, for $T > T_c$, the mobility is higher for GBs with a higher activation energy, in particular it is at maximum for $\varphi = 40.5^\circ$, while for $T < T_c$ the exact $\Sigma 7$ boundary moves fastest (Fig. 2b).

This result explains the apparent contradiction between growth selection experiments and recrystallization experiments. The problem resulted only from the wrong tacit assumption that the pre-exponential factor is essentially independent of misorientation so that only the activation enthalpy controls mobility. Growth selection experiments have to be conducted at very high temperatures (above 600°C), i. e., in the temperature regime, where the mobility of the $40.5^\circ \langle 111 \rangle$ boundary is the highest due to its high pre-exponential factor.

At high temperatures the GB mobility in this angular interval is obviously not dominated by the segregation behaviour of low Σ boundaries. The reason for the changing maximum mobility orientation in different temperature regimes is obviously the orientation dependence of both, the activation enthalpy and the pre-exponential factor. In fact, both are related to each other in a linear fashion (Fig. 9), i. e.,

$$H = a \ln A_0 + \beta \tag{7}$$

where a and β are constants. This correlation is referred to as the compensation effect and will be discussed in Section 4.

The misorientation dependence of GB motion is not confined to pure tilt boundaries. Recent experiments [13] on Al bicrystals with a GB configuration shown in Fig. 3b revealed that the motion of $\langle 111 \rangle$ boundaries in Al in the vicinity of $\Sigma 7$ misorientation depends non-monotonically on the misorientation angle irrespective of the crystallographic configuration of the curved moving boundary, whether pure tilt or mixed tilt-twist. Fig. 4 shows the misorientation dependence of activation parameters for the mo-

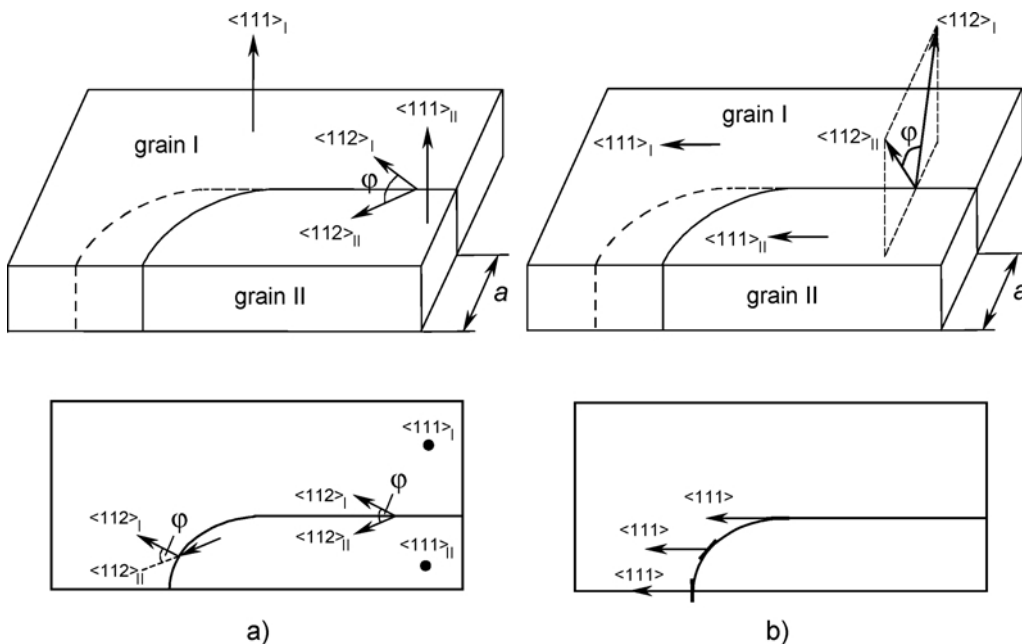


Fig. 3. Bicrystal geometry with the moving curved boundary having (a) pure tilt character and (b) mixed tilt-twist character.

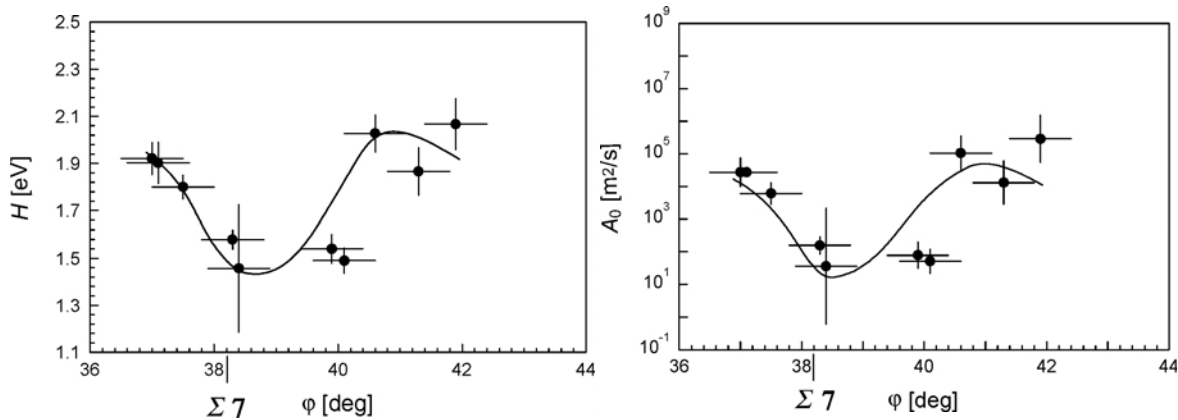


Fig. 4. Activation enthalpy H and pre-exponential factor A_0 for $\langle 111 \rangle$ mixed tilt-twist grain boundaries.

tion of $\langle 111 \rangle$ mixed boundaries [13]. It is seen that both parameters change non-monotonically with misorientation angle and assume a minimum at the $\Sigma 7$ misorientation, which is very similar to the respective misorientation dependence for $\langle 111 \rangle$ tilt boundaries in Fig. 2. Therefore, the curved boundaries in both configurations (Fig. 3), pure tilt with differently inclined boundary elements and mixed tilt-twist, demonstrate essentially the same behaviour with regard to the misorientation dependence of their motion.

One of the principal features of a pure physical experiment is the possibility to analyse experimental results by an independent method, in particular by computer simulation. In Ref. [14] atomistic simulations of the GB motion as a function of temperature and grain boundary misorientation were performed using molecular dynamics for the same geometry, as used in experiment to ensure steady-state, curvature driven boundary migration. These simulations represent the first systematic computational study of the dependence of the GB mobility on misorientation (Fig. 5) and, therefore, probably the only feasible study of the intrinsic (impurity free) boundary mobility since experimentally it is virtually impossible to fabricate bicrystals of perfect purity. Excellent agreement between simulations and experiments was obtained in almost all respects. Specifically, the activation energy and the pre-exponential factor of the boundary mobility exhibited very similar variations with misorientation, including the presence of distinct cusps at low Σ misorientations. It is important to keep in mind that the results of these computer simulations pertain to “absolutely pure material” when discussing the effect of impurity on the orientation dependence of boundary mobility.

3.1. Transition from low- to high-angle boundary

The border between low- and high-angle boundaries is commonly assumed to occur at a misorientation angle of 15° for structural reasons, expressed by Brandon [15]. Recent measurements on stress-driven boundaries can be considered as the first experimental determination of this border afforded by boundary mobility [16]. In Ref. [16] a method to activate and investigate the migration of planar symmetrical and asymmetrical $\langle 111 \rangle$ and $\langle 112 \rangle$ tilt boundaries in Al bicrystals under the action of an external shear stress was introduced. It was shown that low-angle as well as high-angle tilt boundaries can be moved by such shear stress. The transition from low-angle to high-angle $\langle 111 \rangle$ and $\langle 112 \rangle$ boundaries was found to manifest itself as a sharp step of the activation energy at a misorientation angle of $13.6 \pm 0.5^\circ$ which, in the limited framework of experimentally obtained data, seems to be independent of impurity content and tilt boundary plane, but is liable to vary with tilt axis.

3.2. Effect of the boundary plane

GB mobility is known not only to depend on misorientation, but also on the inclination of the GB plane. This is particularly evident for coherent twin boundaries, which are much less mobile than incoherent twin boundaries despite of identical misorientation across the boundary. But anisotropy of GB mobility can also be observed for misorientations other than twin relationships, in particular GBs of a misorientation with $\langle 111 \rangle$ rotation axis. For such orientation re-

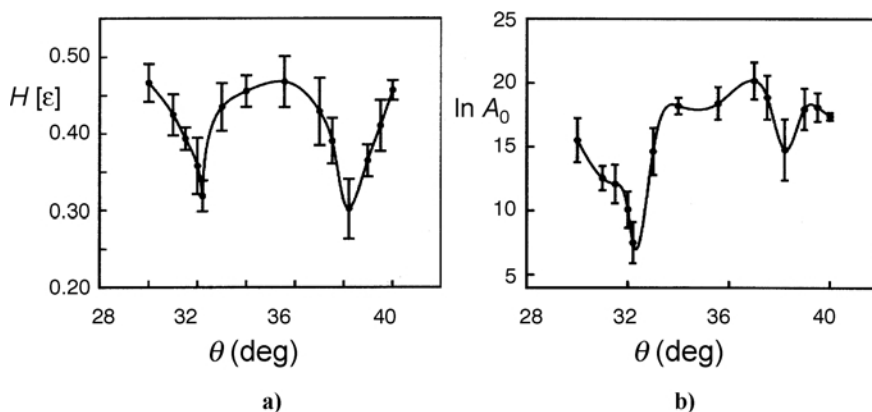


Fig. 5. (a) Activation energy of GB migration ($\epsilon = 0.57$ eV, Lennard–Jones potential well depth for Al) and (b) logarithm of the pre-exponential factor of the reduced mobility as a function of boundary misorientation found in computer simulations of GB motion [14].

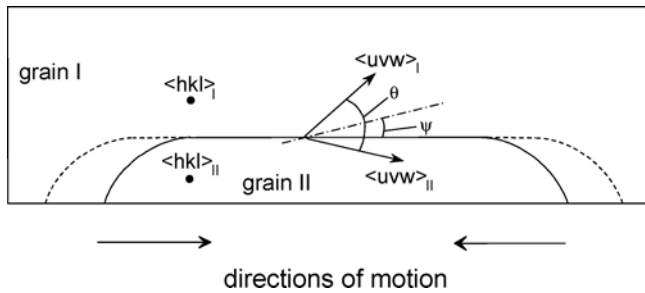


Fig. 6. Motion of curved tilt boundary with different sets of boundary planes. The straight section of the boundary is asymmetrical with an inclination ψ from symmetrical position.

relationships tilt and mixed tilt-twist boundaries can move orders of magnitude faster than pure twist boundaries [17].

In experiments on curved GBs (Fig. 3), the curved part of the boundary consists of crystallographically different boundary planes. If the boundary mobility depends on boundary inclination, this may affect the velocity of steady-state motion of a curved boundary.

In the particular boundary configuration shown in Fig. 3a, the boundary with misorientation angle φ keeps its tilt character with the same angle during its motion. In such experiments [5–7, 11, 12] the average mobility over all differently inclined boundary planes is measured and it is assumed that there is a uniform tilt GB mobility. In fact, it has been recently experimentally confirmed on Al bicrystals, that the change of the set of boundary planes in the curved moving boundary does not affect its motion [13]. This was achieved by using specimens with different inclination of the straight boundary from its symmetrical position. Furthermore, the motion in opposite directions of such a boundary was measured in the same bicrystal, as shown in Fig. 6.

Pure twist boundaries are planar boundaries. Therefore, it is impossible to directly measure their motion by utilizing GB curvature as a driving force. However, a change of the bicrystal geometry provides the opportunity to study the motion of mixed boundaries comprising both tilt and twist components (Fig. 3b). In such a configuration the boundary character changes along its curved part from pure tilt to almost pure twist, although the boundary retains the same misorientation angle φ and axis $\langle 111 \rangle$ of rotation. As mentioned above, the motion of $\langle 111 \rangle$ GBs in configuration Fig. 3b has been studied recently in the angular interval of misorientation between 37 and 42°. Particularly the shape

of the curved moving part of the boundary was measured and compared with the boundary shape which was calculated analytically [18]. The shape of a boundary $y(x)$ (Fig. 7) can be derived from the equation of motion

$$y'' = -\frac{v}{m\sigma_b}y'(1 + (y')^2) \quad (8)$$

assuming that the GB energy σ_b and mobility m are independent of the orientation of the GB relative to the crystallographic axes of the grains. The consistency of measured and calculated boundary shape allows to conclude that different elements of the investigated curved boundary have the same mobility, irrespective of their composition of tilt and twist components. That means an increase of the twist component along the curved mixed boundary in such a geometrical configuration does not affect its steady-state motion.

It is impossible to directly study the effect of GB orientation on its mobility by utilizing the GB curvature as a driving force, since the moving curved part of the boundary consists of different boundary planes. Rather, the motion of flat boundaries has to be investigated. The motion of planar GBs under the action of a magnetic field in bicrystals of a material with anisotropic magnetic susceptibility was investigated in [19, 20]. The experiments were carried out on bicrystals of high-purity bismuth. Symmetrical and asymmetrical ($\psi = 45^\circ$) pure tilt GBs with $90^\circ \langle 112 \rangle$ misorientation were examined. It was found that the motion of asymmetrical boundaries can be very different from symmetrical boundaries. Firstly, the migration activation enthalpy for asymmetrical boundaries is nearly one order of magnitude higher than for a symmetrical one: 3.4–3.8 and 0.51 eV, respectively (Fig. 8a) with a compensation temperature close to the melting temperature of Bi. The most surprising feature is that in contrast to the symmetrical boundary, for an asymmetrical tilt boundary the measured mobility was found to be distinctly different for the motion in opposite directions (Fig. 8b). There are several potential reasons for this anisotropy. First, there is an essential difference in the distance between the crystallographic planes on each side of the boundary. An estimation shows that this factor may change the velocity of GB motion, however, this difference is unlikely to affect the velocity of boundary motion by more than 20 %, which is distinctly less than the observed effect [19]. Second, because boundary motion in Bi bicrystals may be influenced by impurity drag, the difference in the diffusivity of impurities in two opposite directions in the anisotropic structure of Bi should be taken into

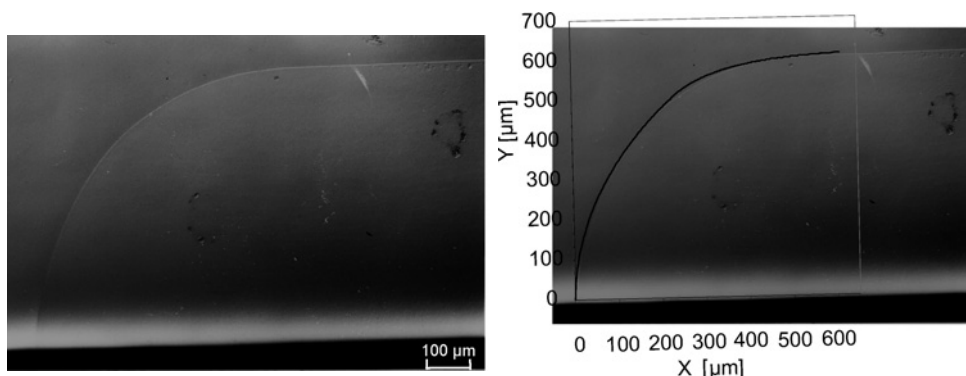


Fig. 7. (a) Measured and (b) calculated shape of a moving $40.6^\circ \langle 111 \rangle$ mixed tilt-twist boundary in pure Al (99.999 %) at $T = 602^\circ\text{C}$.

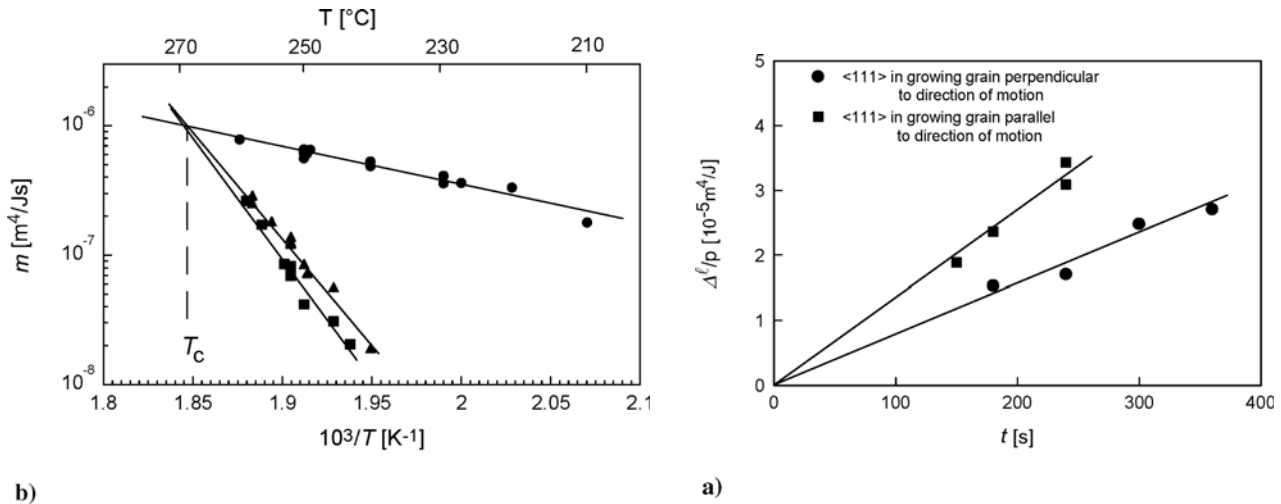


Fig. 8. (a) Temperature dependence of the mobility of 90° $\langle 112 \rangle$ symmetrical (\bullet) and asymmetrical (\blacktriangle , \blacksquare) boundaries in Bi bicrystals, moving in opposite directions [19, 20]. The trigonal axis in the growing grain parallel (\blacktriangle) or perpendicular (\blacksquare) to the growth direction. (b) Displacement Δl (normalized by driving force p) vs. annealing time for asymmetrical tilt boundaries moving in opposite directions.

account. It was shown recently that the motion of a GB in a magnetic field can be considered as a motion of a conductor in a magnetic field, or more strictly, as the motion of a region with a conductivity different from that of the surrounding matrix in a magnetic field. Such a motion causes an electromotive force and, as a consequence, an additional dissipation of energy in a magnetic field [21]. However, the predicted effect is much smaller than experimentally observed. Also this dissipation should, on the one hand, be different for symmetric and asymmetric boundaries and, on the other hand, be different for boundary motion in opposite directions for asymmetric boundaries [21].

In any event, if this asymmetry of GB mobility holds also for other metals, it will have a serious impact on our understanding of GB motion, since the mobility of a GB is commonly conceived as not dependent on its direction of motion.

4. Compensation effect in grain boundary motion

It is well known that the temperature dependence of GB mobility follows an Arrhenius relation (Eq. (5)). Commonly, for evaluation of experimental data the activation en-

thalpy H is determined from the slope H/k of the Arrhenius plot $\ln m$ vs. $1/T$, and much less attention is paid to the pre-exponential factor m_0 . However, there is a large body of experimental evidence that the pre-exponential factor is strongly related to the activation enthalpy: m_0 increases or decreases, if H increases or decreases according to relation (7). This correlation is referred to as the compensation effect, since it strongly moderates the effect of a variation of H on the value of the mobility and, therefore, allows one to use the annealing temperature as a selective tool for grain boundary control.

The compensation effect was repeatedly observed for the mobility of pure tilt boundaries in materials of equal purity [7, 20, 22]. Fig. 6 shows the compensation effect for $\langle 111 \rangle$ tilt boundary migration in the vicinity of the special misorientation $\Sigma 7$. The compensation effect was also observed in molecular dynamics simulations of curved boundary motion [14]. Also, in physical chemistry of surfaces the compensation effect is a common experience and textbook knowledge [23].

A consequence of the specific linear dependence between the activation enthalpy and the logarithm of the pre-expo-

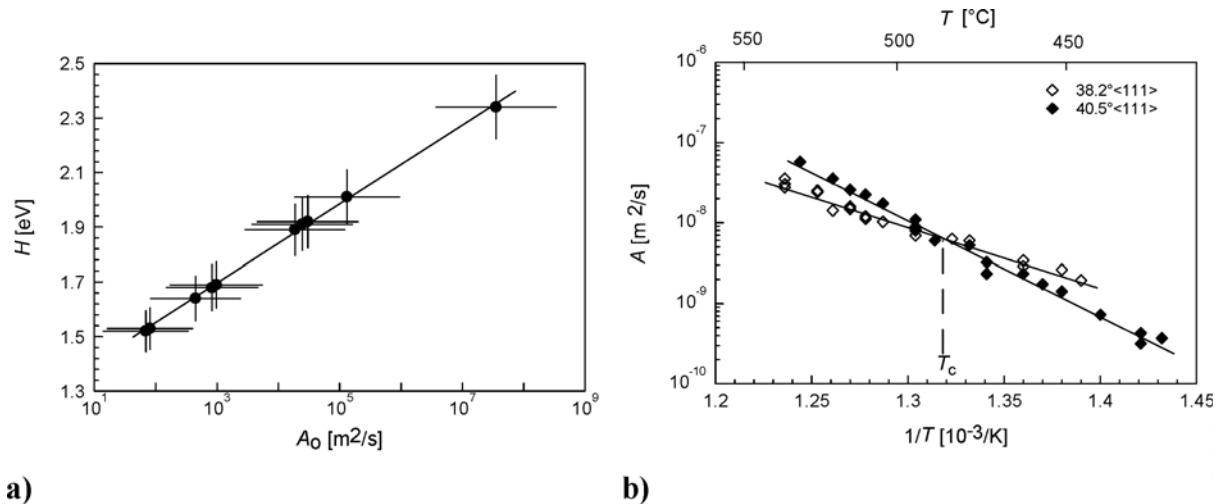


Fig. 9. (a) Dependence of migration activation enthalpy on mobility pre-exponential factor for $\langle 111 \rangle$ tilt GBs in pure Al [12]. (b) Temperature dependence of the reduced mobility A for 38.2° and 40.5° $\langle 111 \rangle$ tilt GBs in pure Al [12].

nential factor is the existence of a so-called compensation temperature $T_c = \alpha/k$, at which the mobilities are equal and at which the kinetic lines in Arrhenius co-ordinates intersect at one point (Fig. 9b). In this context it is worthy to note that the compensation effect was also observed for ^{71}Ge diffusion along $\langle 111 \rangle$ tilt GBs with different angles in the vicinity of the $\Sigma 7$ misorientation in pure Al [24].

The compensation effect can be associated with the fact that the activated state is not a random energy fluctuation in space and time but a defined and thus reproducible although unstable state, which is described by its respective thermodynamic functions [23]. The linear compensation relation and the expression for the compensation temperature can be derived under these conditions. In particular, the compensation temperature can be expressed as

$$T_c = dH/dS|_{\lambda=\lambda_0}$$

where the parameter λ denotes some intensive structural or chemical specification, like angle of misorientation, composition, etc. In this approach T_c is the equilibrium temperature for the activated state.

5. Segregation effects on orientation dependence of boundary mobility

It is well known that the purity of a material has a great influence on GB motion. Impurity atoms almost always reduce the rate of GB migration. However, very little is known on how solute atoms affect GB motion besides the exerted drag, in particular, how impurities influence and thus interact with the GB structure.

The strong interaction of impurities and GB structure is particularly obvious in $\langle 100 \rangle$ tilt boundaries in Al (Fig. 10a). For ultrapure and very impure material the mobility of $\langle 100 \rangle$ tilt boundaries was found to be independent of the rotation angle, irrespective whether special or nonspecial boundary. For intermediate (although high) purity material, the mobility strongly depends on the rotation angle, distinguishing special and nonspecial boundaries. Such a behavior was, however, never reported for tilt boundaries in Al with axis other than $\langle 100 \rangle$.

The common understanding of the orientation dependence of the GB mobility and the effect of solutes on this dependence is mainly founded on results mentioned above [25] as well as on the classical work of Aust and Rutter (Fig. 10b). According to this understanding the orientation dependence of the GB mobility is a segregation effect: strongly ordered boundaries, i.e., low Σ coincidence boundaries segregate less and, therefore, move faster than random boundaries.

This classical concept, however, cannot be confirmed by results of recent experiments [12, 28] and computer simulations [14]. The experimental results reveal that the migration activation enthalpy is strongly affected by both, the boundary crystallography and material purity (Fig. 11). However, in the former case the pre-exponential factor A_0 rises with increasing H by several orders of magnitude, while in the latter case A_0 remains at the same level. Therefore, the pre-exponential factor A_0 in the investigated impurity concentration interval was found to be much less sensitive to the material purity than to a change of the misorientation angle. This result allows to conclude that the observed orientation dependence of mobility (Fig. 2b), deter-

mined by both H and A_0 , does not simply reflect the different segregation behavior of coincidence and random boundaries, as frequently proposed [26, 27], rather it provides evidence for an intrinsic dependence of GB mobility on GB structure. Also molecular dynamics simulations of boundary motion in absolutely pure material reveal strong evidence for the intrinsic structural character of the orientation dependence of boundary mobility [14].

Although the activation enthalpies of both the special and nonspecial boundary depend on impurity concentration (Fig. 11c) they remain vastly different in magnitude with H (random) $>$ H (special). This may be associated with different mechanisms of GB migration irrespective of material purity [28].

Aust and Rutter [27] attributed the abnormally high values of activation enthalpy for GB motion in lead (Fig. 12) to impurity effects on this process and interpreted their results in terms of diffusional mechanisms of boundary motion. However, such an interpretation requires to attribute the difference of activation enthalpy measured for different

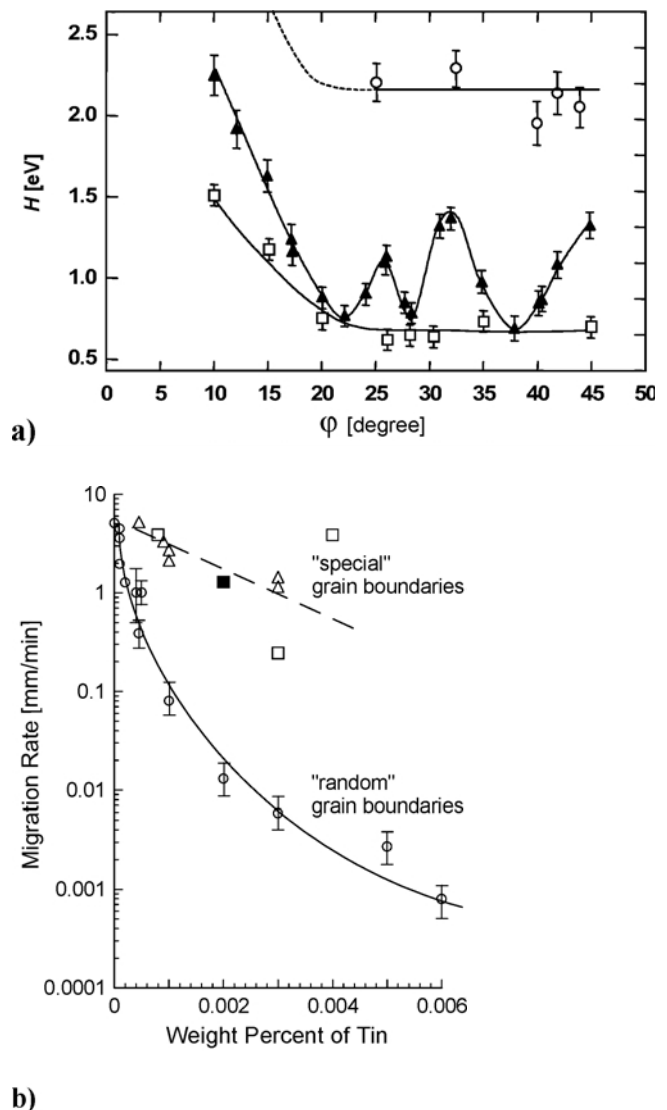


Fig. 10. (a) Dependence of the activation enthalpy of migration for $\langle 100 \rangle$ tilt GBs in Al of different purity: \square -- 99.99995 at%; \blacktriangle -- 99.9992 at%; \circ -- 99.98 at%. [25]. (b) The rate of GB migration vs. the concentration of tin in zone-refined lead at 300 °C [26, 27].

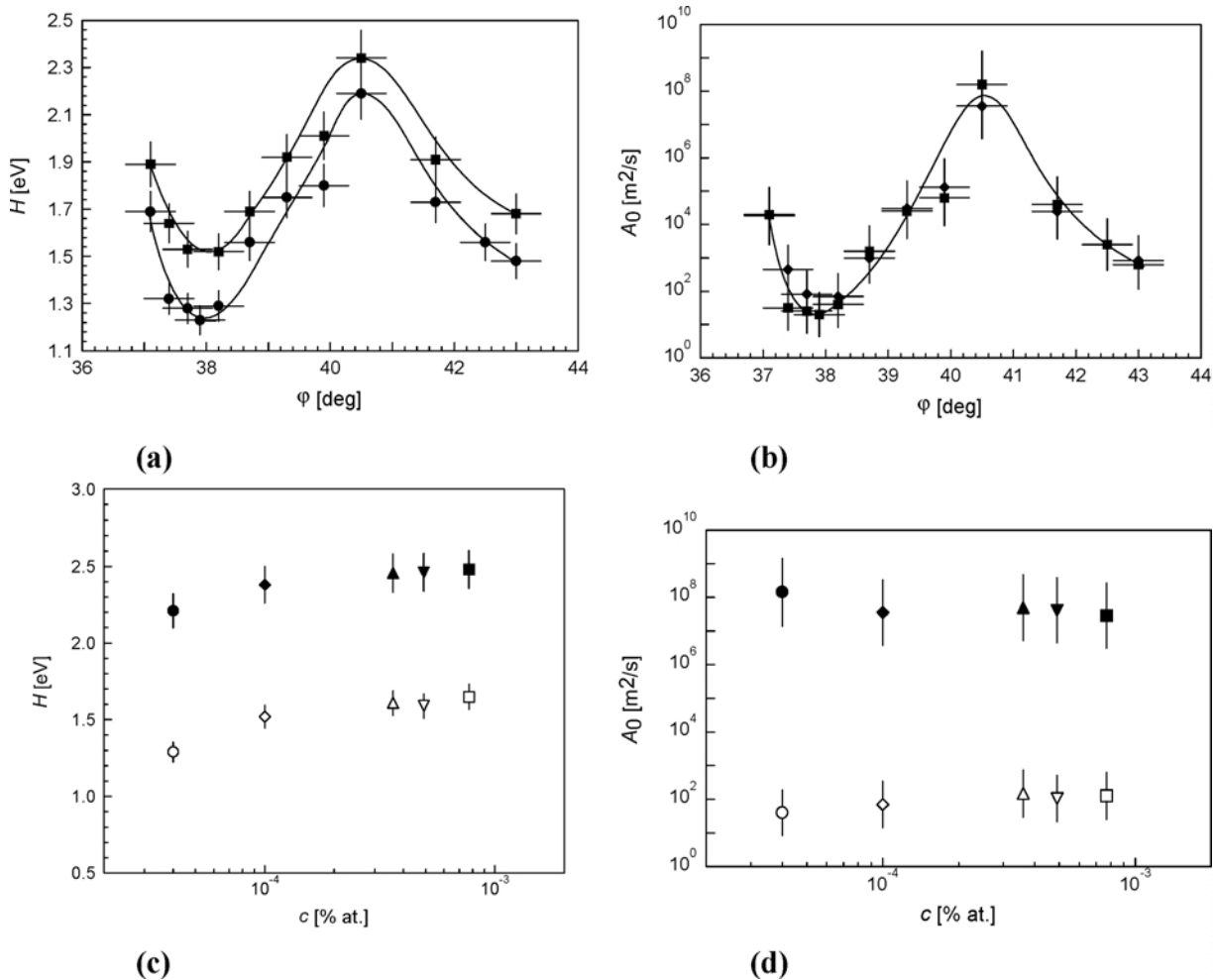


Fig. 11. (a) Activation enthalpy and (b) mobility pre-exponential factor for migration of <111> tilt GBs as a function of misorientation angle for two different Al charges: ● – total impurity concentration $c = 0.4$ ppm; ■ – $c = 1$ ppm. (c) Dependence of activation enthalpy and (d) mobility pre-exponential factor for migration of 38.2° (open symbols) and 40.5° (filled symbols) <111> tilt GBs on impurity concentration in differently pure Al.

boundaries to the adsorption energy of impurity atoms in the pure boundary. This energy normally does not exceed 0.4–0.6 eV [29]. The difference of the activation enthalpy of motion for different boundaries in the experiment of Aust and Rutter amounts to $42.8 - 5.2 = 37.6$ kcal/g–atom (1.63 eV) and, thus, is too large to be interpreted as an adsorption energy of impurities.

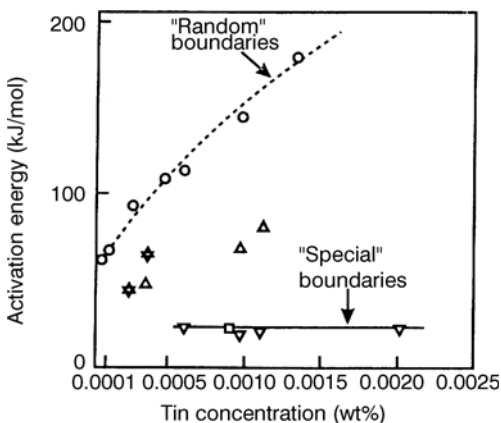


Fig. 12. Measured activation enthalpies vs. tin content in various grain boundaries in zone-refined lead [28].

Moreover, all 17 investigated boundaries in Ref. [27] were crystallographically different and the compensation effect, which obviously reflects the thermodynamic fundamentals of the migration mechanisms for boundaries with different grain misorientation, holds for the migration parameters in the work of Aust and Rutter as well (Fig. 13). The compensation effect for migration of crystallographically different boundaries in lead of almost equal purity (9–13 ppm) in Aust and Rutter's experiment (Fig. 13a) provides unambiguous evidence that the activation parameters do not increase due to an increase of tin concentration in lead, rather than due to different boundary crystallography. The compensation effect is actually observed for migration of all 17 boundaries investigated by Aust and Rutter, irrespective of tin concentration, with a compensation temperature $T_c = 334^\circ\text{C}$ which by practical means is identical with the melting point of Pb (327°C) (Fig. 13b).

6. Dislocation absorption by moving boundaries

An interesting example of the effect of the boundary character on GB control is the influence of dislocation absorption on the migration rate of specific GBs in Al bicrystals. The GB motion in slightly rolled (up to 1.3%) bicrystals

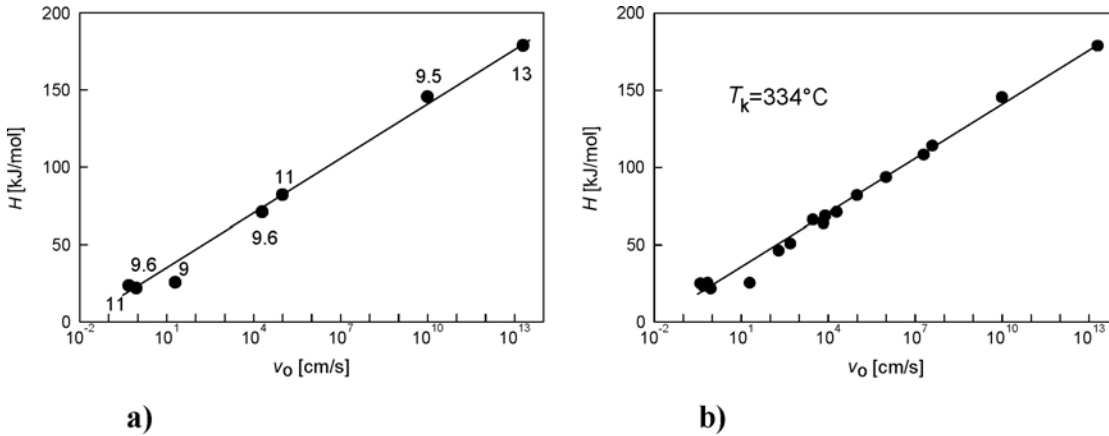


Fig. 13. Relationship between the migration activation enthalpy H and pre-exponential factor v_0 of the velocity equation (Eq. (4)) for migration of GBs in Pb as obtained from an analysis of results of Aust and Rutter [27] (a) for different boundaries in Pb of equal purity (concentration of Sn in Pb in ppm is noted in the figure), and (b) for all 17 measured boundaries in Pb with different crystallography and concentration of Sn from 1 to 13 wt.ppm.

of pure Al (99.999 %) was investigated in [30]. In particular, the migration of $\langle 111 \rangle$ pure tilt GBs and a boundary having an additional twist component (ranging between 5.9° and 9.2°) was measured. In the respective bicrystals the tilt boundary was superimposed by a rotation around the axis perpendicular to the GB plane by an angle ψ . The boundaries moved under the action of a constant capillary driving force provided by the GB surface tension of the curved boundary. For the small strain imposed, the GB mobility was found to decrease substantially with increasing deformation, i.e., increasing density of dislocations for pure tilt (special) boundaries (Fig. 14a). The experiments also showed, however, that for the nontilt (random) boundaries ($40.5^\circ \langle 111 \rangle$ with additional twist components) there was practically no difference in the boundary mobility of deformed and undeformed bicrystals.

Microstructural transmission electron microscopy (TEM) investigations of rolled bicrystals containing a $38^\circ \langle 111 \rangle$ boundary after its migration in a deformed sample reveal the reason for this different behaviour. The pure tilt boundary was always observed to contain extrinsic dislocations (Fig. 14b), apparently swept by the boundary during its migration and not yet absorbed. The presence of these dislocations in the boundary appears to be the reason for a re-

tardation of the boundary migration rate. If the dislocations are only adsorbed in the boundary without being decomposed or annihilated, their stress field – although certainly partly relaxed in the boundary – still contributes to the internal energy and is not released as driving force. In such a case the boundary will not experience the full gain of stored dislocation energy, rather it has to drag along the swept dislocations, which degrades its mobility. Accordingly, random boundaries are obviously more capable of absorbing (annihilating) the swept dislocations than special boundaries. In fact, TEM investigations have shown substantially fewer extrinsic dislocations in the random grain boundaries than in special boundaries [30].

7. Conclusions

The current research on GB dynamics in metals was reviewed. The boundary dynamics, i.e., the boundary reaction to applied forces, is strongly dependent on the GB character, which is commonly reduced to the orientation relationship between adjacent grains and impurity segregation on the boundary.

As shown on specific capillary driven GBs, boundary motion strongly depends on the misorientation angle.

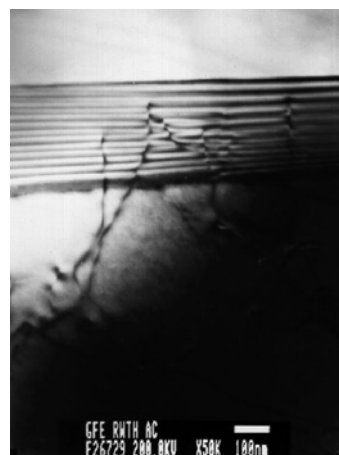
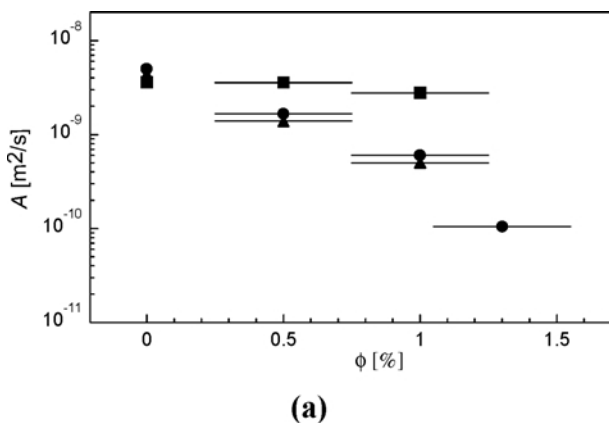


Fig. 14. (a) GB mobility versus degree of rolling ϕ : \bullet – $40.5^\circ \langle 111 \rangle$; \blacktriangle – $37.7^\circ \langle 111 \rangle$; \blacksquare – $40.5^\circ \langle 111 \rangle$ with twist component $5.9^\circ < \psi < 9.2^\circ$. (b) TEM image of moved GB areas in a rolled (1%) bicrystal containing a $38^\circ \langle 111 \rangle$ pure tilt GB.

However, the misorientation dependence of boundary mobility is not confined to pure tilt boundaries. The most recent experiments on Al bicrystals revealed that the motion of $\langle 111 \rangle$ boundaries in Al in the vicinity of $\Sigma 7$ misorientation depends non-monotonically on misorientation angle irrespective of the crystallographic configuration of the curved moving boundary, whether pure tilt or mixed tilt-twist.

In magnetically anisotropic materials GBs can be moved by magnetic forces. Measurements on magnetically driven planar symmetrical and asymmetrical GBs have shown that the inclination of the tilt boundary may have a very strong influence on boundary mobility.

The compensation effect, i. e., the linear correlation between the activation enthalpy and logarithm of the pre-exponential factor, was repeatedly observed for the mobility of GBs in materials of equal purity. A consequence of this dependence is the existence of a compensation temperature, at which the mobilities of different GBs are equal. The compensation effect plays an important role in grain growth and grain structure evolution, since it establishes the relationship between the mobilities of GBs in the granular system at different temperatures.

The purity of a material has a great influence on GB motion. However, the observed orientation dependence of the boundary mobility does not simply reflect the different segregation behavior of coincidence and random boundaries, as frequently proposed, rather it provides evidence for an intrinsic dependence of GB mobility on GB structure. This conclusion is also strongly supported by molecular dynamics simulations of boundary motion in absolutely pure material.

The boundary character also influences dislocation absorption in migrating GBs in Al bicrystals. For pure tilt (special) boundaries the mobility was found to decrease substantially with increasing density of dislocations, while for nontilt (random) boundaries there was practically no difference in the boundary mobility of deformed and undeformed bicrystals.

The authors express their gratitude to the Deutsche Forschungsgemeinschaft for financial support.

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(Received May 14, 2003)

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