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THEORY OF GRAIN BOUNDARY MOTION IN THE PRESENCE OF MOBILE PARTICLES

G. GOTTSTEIN[1] and L. S. SHVINDLERMAN[2]

[1]Institut für Metallkunde und Metallphysik, RWTH Aachen, Kopernikusstr. 14, D-5100 Aachen, Germany and [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia

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Abstract—A theory of grain boundary motion in the presence of mobile particles is put forward. It is shown that the boundary–particle-interaction leads to a hysteresis in the velocity-driving relationship. The extent of the hysteresis depends on particle mobility, which is very sensitive to particle size. The effect of particles is discussed for planar and curved boundaries as well as volume particle distributions. The theory accounts for a smaller limiting grain size during grain growth than predicted by Zener drag. The concept can be generalized to include all kinds of mobile obstacles for boundary migration. In such cases not the distribution of obstacle spacing rather the distribution of obstacle mobilities will control microstructure evolution.

Zusammenfassung—Eine Theorie der Korngrenzenbewegung in Gegenwart beweglicher Teilchen wird vorgestellt. Es wird gezeigt, daß die Wechselwirkung zwischen Korngrenze und Partikel zu einer Hysterese der Beziehung zwischen Korngrenzengeschwindigkeit und treibender Kraft führt. Das Ausmaß der Hysterese hängt über die Teilchenbeweglichkeit sehr empfindlich von der Teilchengröße ab. Der Einfluß von Teilchen wird behandelt für ebene und gekrümmte Korngrenzen sowie für Volumenverteilungen von Teilchen. Die Theorie sagt eine kleinere Endkorngröße bei Kornwachstum voraus als unter alleiniger Berücksichtigung des Zener drags. Das theoretische Konzept kann auf beliebige bewegliche Hindernisse für die Korngrenzenbewegung erweitert werden. In diesem Fall wird die Mikrostrukturentwicklung nicht von der Abstandsverteilung der Teilchen, sondern von der Verteilung der Teilchenbeweglichkeiten bestimmt.

1. INTRODUCTION

The drag by particles of a second phase on a moving grain boundary is traditionally considered in the approximation where the particles act as stationary pinning centers for the boundaries (Zener drag) [1, 2]. Consequently, the effect of particles on grain boundary motion is the more pronounced, the better the dispersion of particles, i.e. the smaller the size of the particles. This is the basis for the control of grain size during grain growth and to a lesser extent also for recrystallization.

On the other hand it has long been known that inclusions in solids are not immobile and that the particle mobility drastically increases with decreasing particle size [3–11]. Therefore, the fundamental assumption that particles remain immobile during recrystallization and grain growth is questionable and liable to cause serious misinterpretations in the technologically interesting limit of fine particle dispersions.

This paper is aimed at an extension of our current theoretical description of grain boundary motion in two-phase materials to include also the influence of particle mobility.

2. OUTLINE OF THEORY

2.1. *Motion of a planar grain boundary*

Let us consider the motion of a planar grain boundary, which is in contact with second phase particles. The velocity of such a boundary is given by

$$v = \Delta F_{\text{eff}} \cdot m_{\text{b}} \tag{1}$$

where m_{b} is the mobility of a grain boundary and ΔF_{eff} is the effective driving force. ΔF_{eff} can be written

$$\Delta F_{\text{eff}} = \Delta F - \sum_i n_i f_i. \tag{2}$$

Here ΔF is the total driving force acting on the grain boundary, n_i is the number of particles with radius r_i per unit area of the boundary, and f_i is the attraction force between the boundary and a particle of size r_i. The value n_i is at present assumed to remain constant during motion, but this assumption will be discussed in more detail in Section 2.6.

On the other hand the velocity of a particle (and therefore also of the boundary in case that both move together) reads according to the Einstein relation

$$v = m_{\text{p}}(r_i) f_i. \tag{3}$$

$m_p(r_i)$ is the mobility of a particle with radius r_i. Combination of equations (1), (2) and (3) yields

$$v = \frac{\Delta F \cdot m_b}{1 + \sum_i n_i \frac{m_b}{m_p(r_i)}} \tag{4}$$

or, for a continuous size distribution of particles per unit area $\bar{n}(r)$

$$v = \frac{\Delta F \cdot m_b}{1 + \int_0^\infty \frac{\bar{n}(r) m_b}{m_p(r)} \mathrm{d}r} \tag{5}$$

with the total number of particles per unit area

$$n = \int_0^\infty \bar{n}(r)\,\mathrm{d}r. \tag{6}$$

Equations (4) or (5) describe in general terms the joint motion of a grain boundary with attached particles. It is evident that the motion of the boundary–particles-complex depends on the mobility of the boundary, mobility of the particles, particles distribution function and, which is particularly important, size of the particles [4–7].

For an estimation of the effect of particle mobility on grain boundary motion we consider two limiting cases.

(I) High particle mobility

$$\int_0^\infty \frac{\bar{n}(r) m_b}{m_p(r)} \mathrm{d}r \ll 1. \tag{7}$$

Then

$$v \cong m_b \Delta F. \tag{8}$$

In this case the grain boundary velocity is determined by the mobility of the boundary.

(II) Low particle mobility

$$\int_0^\infty \frac{\bar{n}(r) m_b}{m_p(r)} \mathrm{d}r \gg 1. \tag{9}$$

Then

$$v \cong \frac{\Delta F}{\int_0^\infty \frac{\bar{n}(r)}{m_p(r)} \mathrm{d}r} \tag{10}$$

or in the simple case of a single size particle distribution [6]: $\bar{n}(r) = n_0 \cdot \delta(r - r_0)$

$$v = \frac{\Delta F m_p(r_0)}{n_0}. \tag{11}$$

In this limit the velocity of the grain boundary is determined by the mobility and the density of the attached particles.

2.2. *Particle mobility*

As mentioned above, the particle mobility depends strongly on particle size. It is obvious that for any kind of atomic transport mechanism that may control particle motion, the particle mobility $m_p(r)$ decreases with increasing size of the particle. As an example, we will consider the mobility of a particle with spherical shape and radius r in case that the atomic transfer is limited by interface diffusion. Then, according to the result given in the Appendix

$$m_p(r) = \frac{\nu_S \Omega^2 D_S}{\pi r^4 kT} \tag{12}$$

where ν_S is the surface density of atoms, Ω the atomic volume and D_S the surface diffusion constant. The mobilities of particles for different atomic transfer mechanisms as derived by several authors are given in Table 1. As can be seen from the table, the particle mobility depends on particle size very strongly for all transfer mechanisms. Therefore, the boundary velocity is most severely influenced by large particles according to equation (10), if their density is appreciable.

If the driving force (per particle) exceeds the critical attraction force f^*, the grain boundary cannot move any longer together with the particles and detaches from them at the velocity

$$v^* = f^* m_p(r) \tag{13}$$

which depends on particle size, of course. The velocity v^* is the highest velocity for the joint movement of particles and grain boundary.

2.3. *Particle–boundary interaction*

In the following we will discuss the nature of the attraction force between particles and grain boundaries. The simplest and commonly exclusively considered attraction force is the well known "Zener-force", which is due to the reduction of grain boundary area by the intersection of particle and boundary. For a spherical particle with radius r and a planar grain boundary, the reduction of grain boundary energy per particle, $\Delta\sigma$ [1] is

$$\Delta\sigma = \sigma(A_1 - \pi r^2) \tag{14}$$

σ denotes the grain boundary surface tension and A_1 the unit area. Correspondingly, the maximum attraction force is

$$f^* = 2\pi r \sigma. \tag{15}$$

A more precise calculation for a flexible boundary gives the Zener force [2, 12]

$$f_z = \tfrac{3}{2}\pi r \sigma. \tag{16}$$

The Zener force, however, is not the only attraction force in a particle–boundary system. For instance, if a particle has a low free energy (surface tension) coherent interface with the matrix, this coherence will be lost, when the particle is swept by the boundary, since the grain boundary migration changes the orientation of the matrix in contact with the particle and, consequently, the interface energy changes by [13]

$$\Delta\sigma = 4\pi r^2(\sigma_2 - \sigma_1) \tag{17}$$

Table 1. Mobility of inclusions in solids

Atomic transport mechanism	Type of inclusion			
	Solid sphere	Spherical bubble	Spherical void	Thermal groove[a]
Bulk diffusion in the matrix (D_{vm})	$m_p(r) \approx \frac{D_{vm}\Omega}{kT}\frac{1}{r^3}$ [6]			$m_g(h) = \frac{3}{2}\frac{\Theta_c \nu_s \Omega^2 D_s}{h^3 kT}$ [4]
	$m_p(r) = \frac{3}{2\pi}\cdot\frac{D_{vm}}{kT}\frac{\Omega^2 C_b}{r^3}$ [11]			
	$m_p(r) = \frac{1}{\pi r^3}\frac{D_{vm}\Omega}{kT}$ [7]			
Bulk diffusion in the inclusion (D_{vi})	$m_p(r) \approx \frac{D_{vi} C_i \Omega^2}{10kT\Omega'}\cdot\frac{1}{r^3}$ [6]		$m_p(r) = \frac{\Gamma}{4\pi}\frac{\Omega^2 P D_{gas}}{(kT)^2 r^3}$ [6]	$m_g(h) = \left(\frac{D_{gas}}{kT}\right)\cdot\left(\frac{P}{kT}\right)\cdot\frac{\Theta_c \Omega^2}{h^2}$ [4]
Interface diffusion (D_S)	$m_p(r) \approx \frac{1}{10}\cdot\frac{D_S a\,\Omega}{kT\,r^4}$ [6]	$m_p(r) = 0.3\left(\frac{a}{r}\right)^4\frac{D_S}{kT}$ [5]		
	$m_p(r) = \frac{a'}{\pi r^4}\frac{D_S\Omega}{kT}$ [7]			
	$m_p(r) = \frac{3}{2\pi}\cdot\frac{\Omega^2}{kT}\cdot\frac{\nu_S D_S}{r^4}$ [11]			
	$m_p(r) = \frac{\nu_S \Omega^2 D_S}{\pi kT r^4}$			
Diffusion of vacancies (D)	$m_p(r) = \frac{3\Gamma'_1 D\Omega}{2\pi f kT}\cdot\frac{1}{r^3}$ [6]			

[a]Mobility per length unit; Θ_c—critical angle in the vertex of the groove; h—depth of the groove; C_b—concentration of diffusing atoms in the bulk; c_i—concentration of diffusing atoms in the inclusion; Ω—atomic volume in the bulk; Ω'—atomic volume in the inclusion; P—pressure inside the void; D_{gas}—diffusion coefficient for the gas inside the void; a—lattice constant; a'—effective thickness of the surface layer; ν_S—density of surface atoms; f—correlation factor; $\Gamma = 1/3\,(1+\nu)/(1-\nu)$; ν—the Poisson ratio; $\Gamma'_1 = 1$ for $l \gg r$; $\Gamma'_1 = \Gamma/3$ for $l \ll r$; l—average distance between source and sink.

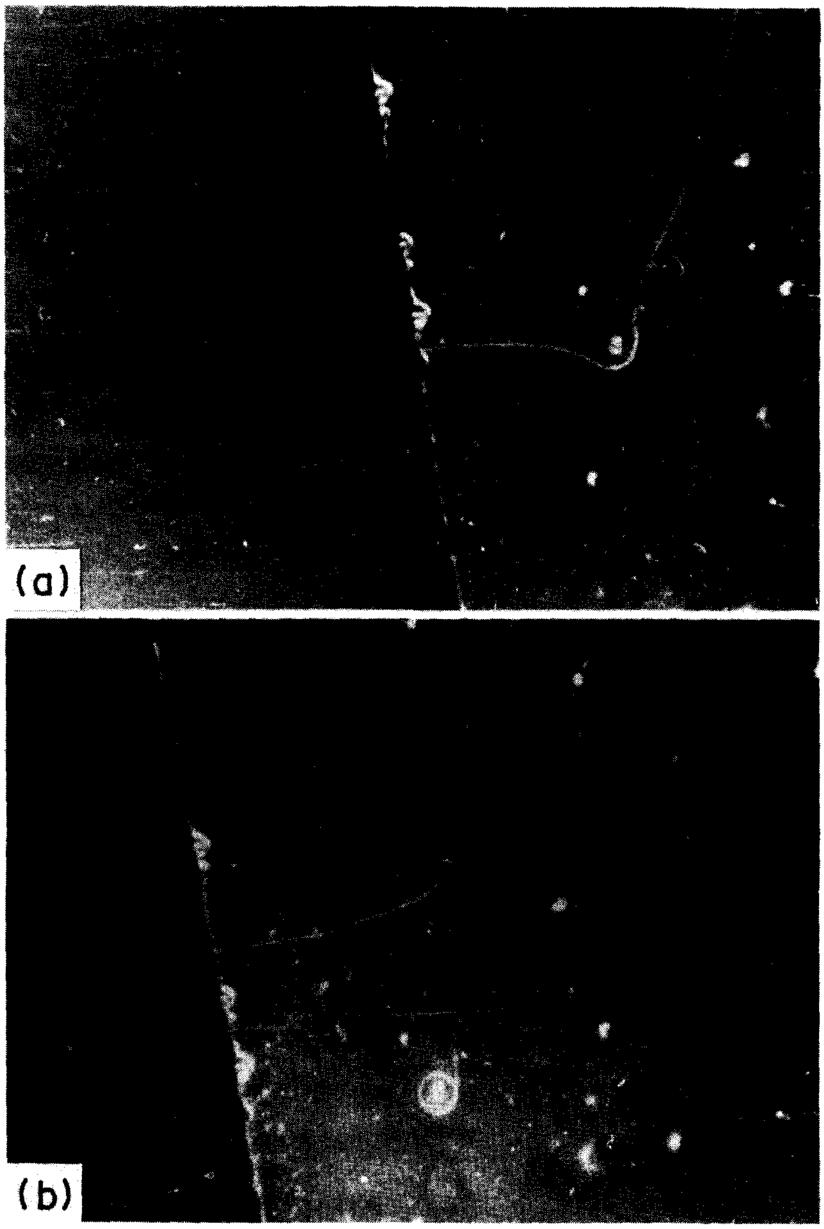

Fig. 1. Example of particle circumvention by a moving grain boundary in copper. (a) Flexing at particle; (b) looping of particle.

and the maximum drag is

$$f_2^* = 8\pi r(\sigma_2 - \sigma_1) \tag{18}$$

where σ_1, σ_2 are the interface energies of the particles in the growing and vanishing grain, respectively.

If the increase of interface energy according to equation (17) exceeds a critical value, then the moving grain boundary prefers to circumvent the particle and to leave behind a spherical volume of the original grain with the particle inside [8]. In this case (Fig. 1)

$$\Delta\sigma = 4\pi r^2\sigma \tag{19}$$

and the maximum attraction force

$$f_3^* = 8\pi r\sigma. \tag{20}$$

The maximum attraction force will be determined by the respective particle boundary interaction, according to equations (16), (18) or (20) and will control the detachment of the grain boundary from the particles.

2.4. Velocity–driving force relationship

The collective movement of particles and grain boundary at subcritical driving forces, and the detachment of particles at supercritical driving forces results in a bifurcation of the grain boundary migration rate with increasing driving force. For a single size particle distribution this is schematically shown in Fig. 2. At low driving forces ΔF, the boundary moves together with the particles and the kinetics of

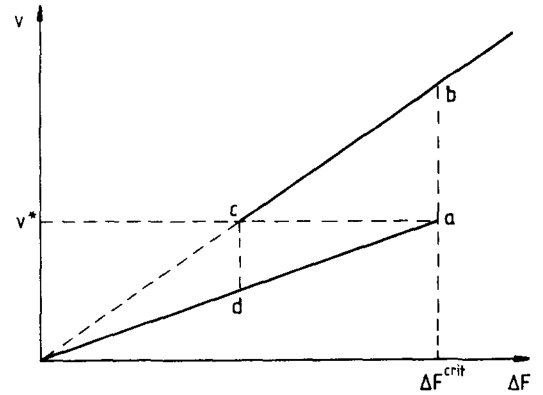

Fig. 2. Schematic dependency of grain boundary velocity on driving force for a single size particle distribution on the boundary. ΔF^{crit} is the Zener force. The behavior is discontinuous at ΔF^* and v^*.

this movement are determined by the particle mobility and density [equation (11)]. When the driving force reaches the critical value $\Delta F^{crit} = f^* \cdot n$, the grain boundary will break away from the particles, and thus, instantly increase its velocity to the migration rate of an unloaded boundary (point b in Fig. 2). The velocity difference between a loaded and a free boundary corresponds to the difference between the particle mobility $[m_p(r)/n]$ and grain boundary mobility (m_b). On the other hand, if the driving force ΔF acting on an unloaded boundary decreases, the grain boundary velocity will decrease in proportion to the driving force until a critical value v^* (point c in Fig. 2) is reached. At this point the boundary velocity changes discontinuously to the velocity corresponding to the loaded boundary, since then the particles become capable of moving with the boundary and will exert a drag force. Therefore, a hysteresis exists between the points of particle detachment with increasing driving force and particle attachment at decreasing boundary velocity. The gap between the critical points—the size of the hysteresis—is for a single size particle distribution

$$\Delta F_a - \Delta F_c = f^* n \left(1 - \frac{m_p(r)}{n m_b}\right) \tag{21}$$

i.e. it rises with increasing critical attraction force f^*, density of particles n and mobility ratio $n \cdot m_b/m_p(r)$.

In real systems, the relation will be more complicated, since the particles will not be of uniform size, but will have a size distribution, and the normalized particle mobility $m_p(r)/n$ and thus, the hysteresis, will depend on the shape of distribution function according to equation (5) (see Section 2.6).

2.5. *Effect of boundary curvature*

So far we have tacitly assumed that the grain boundary remains planar during motion. In real processes, however, like recrystallization and grain growth, boundaries will be curved and, therefore, the curvature has to be taken into account.

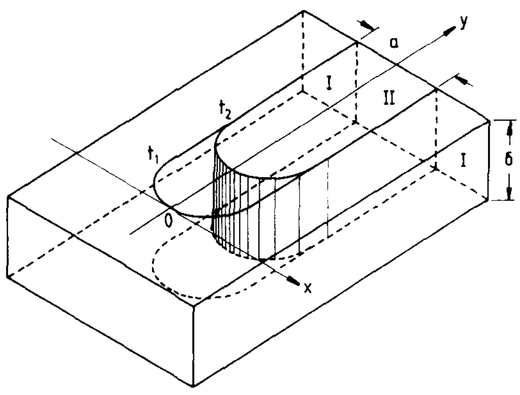

Fig. 3. Sketch of bicrystal geometry for a moving grain boundary half-loop.

Here we will treat the effect of curvature on the acting driving force and, correspondingly, on the particle detachment/attachment process, which is relevant in particular for grain boundary motion during grain growth. We shall confine our consideration to the steady state motion of a grain boundary half-loop [14–16]. This choice has the advantage that the shape and character of a grain boundary half-loop during steady state motion can be described analytically. On the other hand, the consideration can, in principle, be extended to more complex geometries without requiring an extension of the underlying physical concepts.

For sake of simplicity let us consider the steady state motion of a grain boundary (Fig. 3) in a system with a single size particle distribution. The shape of a half-loop $y = \Phi(x)$ (Fig. 4) during its steady state motion can be described in a coordinate system attached to the moving boundary by [16]

$$\Phi'' = -\frac{V}{\sigma m_b} \Phi'[1 + (\Phi')^2] \tag{22}$$

where V is the displacement rate of the half-loop moving as a whole and σ the grain boundary surface tension, which we assume not to change with grain

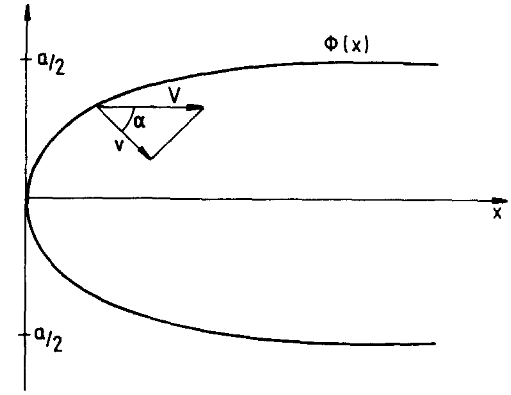

Fig. 4. Relation between overall half-loop velocity V and velocity v of arbitrary grain boundary segment.

boundary orientation in the following case. The general solution of equation (22) reads [16]

$$\Phi(x) = \Phi_0 + \frac{m_b \sigma}{V} \arccos(e^{(-(X - X_0)\cdot V)/(m_b \cdot \sigma)}) \quad (23)$$

and with the initial configuration (at $t = 0$) of a half-loop with radius $a/2$ and vertex at $x = 0$

$$\Phi = \frac{a}{\pi} \arccos e^{-(\pi x)/a} \quad (24a)$$

$$V = \frac{\pi \sigma m_b}{a} = \frac{2\sigma}{a} \cdot \frac{\pi m_b}{2} \quad (24b)$$

where $2\sigma/a$ corresponds to the average driving force and $\pi m_b/2$ to the average half-loop mobility.

The index "L" denotes loaded boundary. The free moving part in vicinity of the vertex assumes the shape Φ_F (F for free boundary)

$$\Phi_F = \Phi_{0F} + \frac{m_{bf}\sigma}{V} \arccos(e^{(-(x - x_{0F})\cdot V)/(m_{bf}\cdot\sigma)}). \quad (28)$$

Correspondingly, there is a point x^* where

$$\Phi_L(x^*) = \Phi_F(x^*); \quad \Phi'_L(x^*) = \Phi'_F(x^*) \quad (29)$$

since the boundary cannot have discontinuities or kinks.

With the initial conditions: $\Phi_F(0) = 0$, $\Phi_L(\infty) = a/2$ and $\Phi'_F(0) = \infty$, we obtain the general solution

$$\Phi(x) = \begin{cases} \frac{m_{bf}\sigma}{V} \arccos\left(\exp - \frac{Vx}{m_{bf}\sigma}\right) & 0 \leqslant x \leqslant x^* \\ \frac{a}{2} - \frac{m_p(r)}{n}\frac{\sigma}{V} \arcsin\left(\exp - \frac{\left[x - x^*\left(1 - \frac{m_p(r)}{n m_{bf}}\right)\right] Vn}{m_p(r)\sigma}\right) & x \geqslant x^* \end{cases} \quad (30)$$

The actual form of the solution depends on how the mobility m_b and boundary surface tension σ change locally. Since the mobility m_b is determined either by the particle mobility $m_p(r)/n$ or by the mobility of the free boundary m_{bf}

$$m_b = \frac{m_p(r)}{n} + \Theta(v - v^*)\left[m_{bf} - \frac{m_p(r)}{n}\right] \quad (25)$$

where Θ is the Heaviside step function and v^* the critical velocity, where the transition from a free moving boundary to a boundary loaded with particles occurs. While the half-loop is displaced with constant velocity V parallel to itself, the individual sections of the grain boundary move parallel to the grain boundary normal of this section with velocity (Fig. 4)

$$v = V \cos \alpha = V\Phi'[1 + (\Phi')^2]^{-1/2}. \quad (26)$$

Therefore, the grain boundary velocity changes locally: it is at its maximum at the vertex of the half-loop, but drops to zero at the loop section parallel to the X-axis.

If the vertex velocity $V < v^*$, then the bounary does not become detached from the particles at any point, hence its mobility $m_b = m_p(r)/n = \text{const.}$, and its shape and velocity are described by equations (24).

If $V > v^*$, then the vertex moves freely with mobility m_{bf}, but there will always be a section of the half-loop, where $V < v^*$, i.e. where the particles and the boundary move together with mobility $m_p(r)/n$. The shape Φ_L of this latter part is determined by an expression similar to equation (23)

$$\Phi_L = \Phi_{0L} + \frac{m_p(r)}{n}\frac{\sigma}{V} \arccos(e^{(-(x - x_{0L})\cdot Vn)/(\sigma \cdot m_p(r))}). \quad (27)$$

where

$$x^* = \frac{m_{bf}\sigma}{V} \ln \frac{V}{v^*} \quad (31)$$

$$v^* = V \sin\left(\frac{\pi}{2}\frac{V_F - V}{V_F - V_L}\right). \quad (32)$$

Also

$$V_F = \frac{\pi \sigma m_{bf}}{a} \quad (33a)$$

$$V_L = \frac{\pi\sigma}{a}\frac{m_p(r)}{n}. \quad (33b)$$

The change in shape of the half-loop on break-away from the particles is given schematically in Fig. 5. It is emphasized that the detachment from the particles must flatten the moving grain boundary. This result is in a good agreement with experimental data [11]. The dependence $v^*(V)$ according to equation (32) is shown in Fig. 6 for various ratios $\alpha = V_L/V_F$. For $\alpha = 0.5$ the behavior of the half-loop is shown in bold lines. If v^*/V is large, then the boundary moves together with the particles and its velocity is

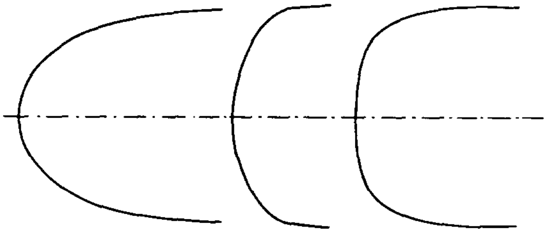

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Fig. 5. Shape change of a grain boundary half-loop during detachment from particles. (a) before detachment, (b, c) progressive stages of detachment.

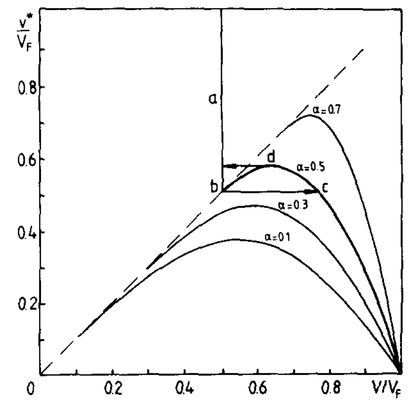

Fig. 6. Steady state half-loop velocity for different ratios $\alpha = V_L/V_F$ according to equation (32) (see text for details).

$V_L = \pi\sigma m_p(r)/(na)$ (line a–b in Fig. 6). If the ratio v^*/V_F decreases to reach $v^*/V_F = \alpha$, some of the particles detach from the half-loop vertex and the boundary velocity discontinuously changes to point "c" (Fig. 6). With further reduction of v^*/V more and more particles break away from the half-loop and its velocity approaches V_F. Conversely, if v^*/V_F increases, the half-loop velocity follows the same curve to the point "d" and then discontinuously changes to $V_L = \pi\sigma m_p(r)/(na)$, because of particle attachment. As a result, also for a curved boundary a hysteresis effect is obtained, similar to the behavior of a planar grain boundary.

2.6. *Grain boundary motion in a particle containing volume*

So far we have considered the migration of a boundary loaded with particles and the velocity dependent detachment of particles from the boundary. In reality, however, there will be a volume distribution of particles, and we define the particle volume distribution function $\bar{n}_v(r)\,dr$ as the number of particles per unit volume with size between r and $r + dr$.

For a stationary boundary ($v = 0$) an equilibrium distribution of particles on the boundary $\bar{n}_b(r)$ will be established, which is different from the volume distribution owing to the interaction energy $\Delta F_z = k_1\pi r^2\sigma$, between particle and boundary (the Zener energy, k_1—geometry factor)

$$\bar{n}_b(r)\,dr = \bar{n}_V(r)2r\,\exp\left(+\frac{k_1\cdot\pi r^2\sigma}{kT}\right)dr. \quad (34)$$

If a boundary would move from a particle free volume to a particle containing volume, the equilibrium distribution will be readily established, since the influx of particles per unit area $\Delta n^+ = \bar{n}_v v\Delta t$ during the time interval $\Delta t = \Delta x/v$, where Δx is the boundary displacement, is balanced by the loss rate $\Delta n^- = n_b(r)/\tau^-(r)$ where $\tau^-(r)$ is the average "life" time of a particle of size r in the boundary. If $\tau^-(r) < d(r)/v$, where $d(r)$ is the average spacing of particles with size r, the thermal equilibrium distribution $\bar{n}_b(r)$ is maintained during boundary migration. In the following we shall assume that this condition holds†.

For a moving boundary, however, the equilibrium particle distribution can be only maintained for particles, which are able to migrate with the boundary, i.e. for a given velocity only all particles with size $r < r_c(v)$. At an instant of time, a moving boundary will, therefore, be in contact with two types of particles, namely the thermally distributed particles for $r < r_c(v)$ and the volume distribution of particles with $r > r_c(v)$, to which the boundary is attached temporarily during its motion. The total number of particles per unit area on a boundary moving with velocity v is

$$N_{tot} = \int_0^{r_c} \bar{n}_b(r)\,dr + \int_{r_c}^{\infty} \bar{n}_v(r)2r\,dr. \quad (35)$$

Both kinds of particles, however, have quite a different effect on boundary migration. While the small particles, which migrate with the boundary, reduce the effective driving force, owing to their drag as demonstrated in Section 2.1, the large statistically touched particles constitute a frictional force, which determines the mobility of a free moving boundary in a volume containing a particle distribution $\bar{n}_v(r)$, $r > r_c$.

With increasing boundary velocity the number of particles attached to the boundary diminishes so that the net drag effect decreases, while the frictional forces increase owing to a growing number of contacted but unattached particles. Therefore, the dependence of boundary velocity on driving force does not reveal a discontinuity as in Fig. 2, rather it will continuously change between the two branches pertaining to the loaded and free moving boundary (lower curve in Fig. 7). Conversely, if the boundary slows down, more and more particles with

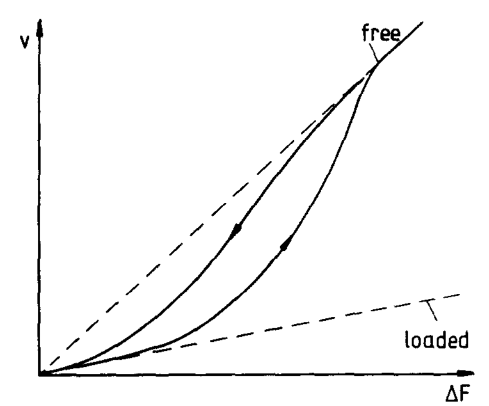

Fig. 7. Schematic dependency of grain boundary velocity on driving force for grain boundary motion through a particle containing volume.

†This assumption does not limit the general validity of the conclusions. In case of $\tau \geq d(r)/v$, the boundary distribution would attain a higher density, but nevertheless constant particle distribution, since the thermal particle loss rate increases with particle density.

increasing size become attached to the boundary. However, the velocity where a particle becomes attached to a more freely moving boundary is attained at a lower driving force than the one at which particles of the same size became detached from the more loaded boundary (upper curve in Fig. 7). Therefore, a hysteresis of $v(\Delta F)$ is also obtained from grain boundary motion in a particle containing volume, and qualitatively the same conclusions hold as for a particle containing boundary in a pure single phase crystal, as treated in Section 2.1.

3. DISCUSSION

3.1. The limiting grain size during grain growth

Particle drag will always affect grain boundary motion in two phase systems except at driving forces high enough to completely detach particles from the boundary. Pronounced effects ought to be expected for cases, where a transition from a free to a loaded boundary occurs. This is likely to happen, if the driving force drops or grain boundary migration slows down during the process like during continuous grain growth or even primary recrystallization with concurrent strong recovery. The net effect of particle drag on grain growth ought to be slower kinetics and a final grain size smaller than predicted by the Zener drag. It would be difficult to extract the particle influence on grain growth kinetics, since no difference in the time exponent of grain growth kinetics is expected as long as the boundary moves entirely free or fully loaded. However, the activation energy ought to be different from particle drag controlled motion, since then the boundary migration rate is controlled by the particle mobility, which is likely to have an activation energy different from the mechanism of grain boundary motion. However, there is little data about the diffusivitiy in particle/matrix interfaces, hence there is no unambiguous distinction between the processes from the value of the activation energy. For more information on the controlling mechanisms it would be necessary to conduct boundary migration experiments in bicrystals at different temperatures and pressures, i.e. to determine both the activation energy and the activation volume of the controlling process.

There ought to be a noticeable influence on the final grain size, however. According to Zener the final grain size (radius R_f) is obtained when the Zener drag force $3f\gamma/(2r_p)$ balances the driving force $2\gamma/R_f$, hence $R_f = 4r_p/(3f)$. Usually, this is not observed in grain growth experiments, rather the final grain size for continuous grain growth is found considerably smaller than predicted by Zener [17]. This can be readily understood from particle drag, in terms of Fig. 7. At large driving forces the boundary moves essentially freely. With increasing average grain size the driving force decreases and the grain boundaries slow down. Eventually they will be moving slowly enough to be caught up by the particles. This drastically reduces the boundary migration rate, which although theoretically finite, will become unmeasurably small. Since the boundary is loaded with particles, it will cease to move at a much smaller grain size than predicted by Zener.

3.2. The generalized drag concept

The theory presented for particle drag is very akin to the solute drag theory, developed some thirty years ago for the drag by solute atoms on grain boundaries in impure materials [18–20]. In fact, the solute drag theory in its most simple form exactly corresponds to the particle drag theory with the particle size corresponding to the size of a solute atom. The drag, however, is not confined to spherical or differently shaped foreign constituents. Equally, surface grooves can be dragged along and will exert respective retarding forces on the boundary. Therefore, the particle drag concept can be extended to any mobile obstacle of grain boundary motion, and, in general, there will always be a wide variety of obstacles, including solute atoms, particles of different size and coherency and eventually, surface grooves.

When considering the net effect of these obstacles on grain boundary motion and therefore, basically for microstructure development, there is a major difference to the current understanding of static obstacle–boundary interference. The impact of immobile obstacles on microstructure evolution is essentially described by the distribution of their spacing. In the more generalized concept of mobile obstacles, it is not the distribution of their spacing rather it is the distribution of their mobilities that controls their interaction with lattice defects like grain boundaries and, therefore, microstructure development. As a matter of fact, these two approaches although seemingly similar, are quite different in their influence. While the static distribution of immobile obstacles invariably determines the interaction and final microstructure under any external condition, the mobility of obstacles is far from being constant, rather it will depend strongly on temperature, and the mechanism of migration may change with size, geometry and composition of the obstacles as well as temperature. Of course, this complicates considerably the description of microstructure evolution, but at the same time, it will open the spectrum of variety and, therefore, flexible microstructure control.

4. CONCLUSIONS

1. A theory of grain boundary motion in systems with mobile particles is put forward. Different mechanisms of grain boundary–particle interaction and the corresponding attraction forces are introduced.

2. The boundary migration behavior can be discussed in terms of the dimensionless parameter

$$\beta = \int_0^{\infty} \frac{\bar{n}(r)m_b}{m_p(r)}\,dr.$$

For $\beta \ll 1$ (small particles) boundary motion is controlled by boundary mobility (m_b), but for $\beta \gg 1$ (large particles) the boundary velocity is determined by particle density $\bar{n}(r)$ and particle mobility $m_p(r)$.
3. Particles can detach from the boundary, if the driving force exceeds the attraction force, but can be reattached to the boundary when the boundary velocity drops below a critical value. The points of detachment and attachment are not identical, giving rise to a hysteresis.
4. Due to this hysteresis, a curved grain boundary tends to flatten under the influence of particle drag.
5. The theory can be qualitatively extended to a volume distribution of particles. In this case the velocity–driving force dependency is not linear any more, but still exhibits a hysteresis.
6. The theory can qualitatively account for the observed deviation of final grain size during grain growth from the Zener approximation.
7. The theory can be generalized to all kinds of mobile obstacles, including solute atoms and thermal grooves. For mobile obstacles, grain boundary behavior and eventually microstructure evolution is not any more determined by the distribution of *obstacle spacing*, rather than by the distribution of *obstacle mobilities*.

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APPENDIX

As an example we will determine the mobility of a particle of spherical shape (radius r) when the atomic transfer is limited by surface (interface) diffusion. We use the approach given in [4] where the equation of balance of the free energy was found from the condition that the work completed in a unit of time on the side of the boundary above the particle due to the influence of the force, has to equal the energy dissipated by single atoms

$$\Delta F \cdot V = \int_S f_a V_a v_S \,dx\,dz \qquad \text{(A1)}$$

where V is the velocity of the particle, $f_a(x)$ is the thermodynamic force affecting a single atom at points of the surface with coordinate x, z; V_a is the diffusion velocity of the atoms, v_S is the surface density of atoms, S is the integration path. For a homogeneous isotropic surface ($v_S = \text{const}$, D_S—the diffusion coefficient does not depend on coordinates) and allowing for the Einstein equation yields

$$\Delta F \cdot V = \frac{v_S kT}{D_S} \int_{-\sqrt{r^2-x^2}}^{\sqrt{r^2-x^2}} \int_{-r}^{r} V_a^2 \,dx\,dz. \qquad \text{(A2)}$$

The velocity V is related to the rate at which the interface $y(x, z)$ bends itself

$$v_S \Omega \frac{\partial V_a}{\partial x} = -\frac{\partial y}{\partial t}\left[1 + \left[\frac{\partial y}{\partial x}\right]^2\right]^{1/2} \cong -\frac{\partial y}{\partial t} = \frac{\partial y}{\partial x}\frac{\partial x}{\partial t} = \frac{\partial y}{\partial x} V \qquad \text{(A3)}$$

Ω is the atomic volume.

Since $V_a(\pm\infty, t) = 0$ and $y(\pm\infty, t) = 0$, the mobility of the particle will be

$$m_p(r) = \frac{v_S \Omega^2 D_S}{kT}\left[\int_{-\sqrt{r^2-x^2}}^{\sqrt{r^2-x^2}} \int_{-r}^{r} y^2 \,dx\,dz\right]^{-1} = \frac{v_S \Omega^2 D_S}{\pi r^4 kT}. \qquad \text{(A4)}$$