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Triple junction drag and grain growth in 2D polycrystals

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Abstract

The process of grain growth in 2D systems is analyzed with respect to the controlling kinetics: from solely boundary kinetics, when grain growth in a polycrystal is determined by the Von Neumann–Mullins relation, to exclusively triple junction kinetics, when grain growth is governed by the mobility of triple junctions. It is shown that in the "intermediate" case, when the driving force for grain boundary motion and the characteristic mobility are grain boundary curvature and grain boundary mobility, respectively, a limited mobility of triple junctions essentially influences grain boundary motion. The Von Neumann–Mullins relation does not hold anymore, and this is the more pronounced the smaller the triple junction mobility. In the case where grain growth is determined by the mobility of grain boundary triple junctions (triple junction kinetics) all grains are transformed into polygons in the course of grain growth. Grain growth would cease if all grains assumed the shape of regular polygons, not only hexagons like in the Von Neumann–Mullins case. The only exceptions are triangles: they collapse without transforming into a polygon. The respective relation for the rate of a change of grain area under triple junction kinetics is obtained and discussed with regard to microstructure evolution. © 2002 Acta Materialia Inc. Published by Elsevier Science Ltd. All rights reserved.

Keywords: Grain growth; Kinetics; 2D polycrystals

1. Introduction

The Von Neumann–Mullins relation [1,2] constitutes a basis for practically all theoretical and experimental investigations as well as computer simulations of microstructural evolution in 2D polycrystals in the course of grain growth [3–5]. One of the principal features underlying this relation is the assumption that the triple junctions do not drag grain boundary motion. However, several recent theoretical and experimental studies provide evidence that the kinetics of triple junctions may be different from the kinetics of the adjoining grain boundaries [6–11]. This affects the kinetics of microstructure evolution during grain growth. In the present work we will consider firstly grain boundary motion, or, more correctly, the change of area of a specific 2D grain under the condition that despite a strong influence of triple junctions, the evolution of the system is controlled by grain boundary motion. In the second part the microstructural evolution of 2D polycrystals will be considered under the condition that the motion

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of a grain boundary system with triple junctions is controlled by triple junction kinetics. The consideration in both the first and the second part will be conducted under the assumptions [6,9,11] that the system migrates under the action of the surface tension of uniform grain boundaries only, in other words, the average grain growth process is considered. In the second part of the paper we will consider microstructure evolution of 2D polycrystals during grain growth under triple junction kinetics, and we will show that for the kinetics not only grain boundary mobility m_b and triple junction mobility m_{tj} but also the grain size plays a role.

2. The Von Neumann–Mullins relation

For grain growth in a 2D system, Mullins [2] derived a fundamental relation, which was originally formulated by Von Neumann for 2D soap froth [1]. The respective model makes very fundamental assumptions, namely: (1) all grain boundaries possess equal mobilities and surface tensions, irrespective of their misorientation and the crystallographic orientations of the boundaries; (2) the mobility of a grain boundary is independent of its velocity; (3) the triple junctions do not affect grain boundary motion; therefore, the contact angles at triple junctions are always in equilibrium and, due to the first assumption, are equal to 120°.

Let us consider a 2D grain with an area S [12]. In the time interval dt all points on the grain boundaries of the considered grain will displace normal to the grain boundaries by the amount V dt, where V is the grain boundary migration rate. Accordingly, the rate of change of the grain area S can be expressed by

$$\frac{dS}{dt} = -\oint V\,dl \tag{1}$$

where dl is an element of the grain perimeter. For grain growth

$$V = \sigma m_b K \equiv A_b K \tag{2}$$

where m_b is the grain boundary mobility, σ is the grain boundary surface tension. K is the local curvature of the grain boundary

$$K = \frac{d\varphi}{dl} \tag{3}$$

where φ is the tangential angle at any given point of the grain boundary.

From equations (1)–(3) follows

$$\frac{dS}{dt} = -A_b \oint d\varphi \tag{4}$$

If the grain were bordered by a smooth line, the integral in Eq. (4) would equal 2π. However, owing to the discontinuous angular change at every triple junction, the angular interval $\Delta\varphi=\pi/3$ is subtracted from the total value 2π for each triple junction. Consequently

$$\frac{dS}{dt} = -A_b\left(2\pi - \frac{n\pi}{3}\right) = \frac{A_b\pi}{3}(n-6) \tag{5}$$

where n is the number of triple junctions for each respective grain, i.e. the topological class of the grain. Thus, the rate of area change is independent of the shape of the boundaries and determined by the topological class n only. Grains with $n>6$ will grow and those with $n<6$ will disappear [2].

3. Grain boundary motion dragged by triple junctions

3.1. *Vertex angle for **n**<6*

Evidently, the existence of triple junctions markedly affects the kinetics of grain growth. However, we will show below that the interaction of moving grain boundaries with triple junctions also drastically affects our conception of microstructure evolution. A comprehensive treatment for grain boundary motion controlled grain growth affected by triple junction drag has been given in [6–9]. For a comparison with grain growth controlled by triple junction motion, the major results will be reiterated below.Fig. 1

An analysis of the steady state motion of model grain boundary systems helps us to understand the influence of the mobility of a triple junction on the migration of grain boundaries in polycrystals. In

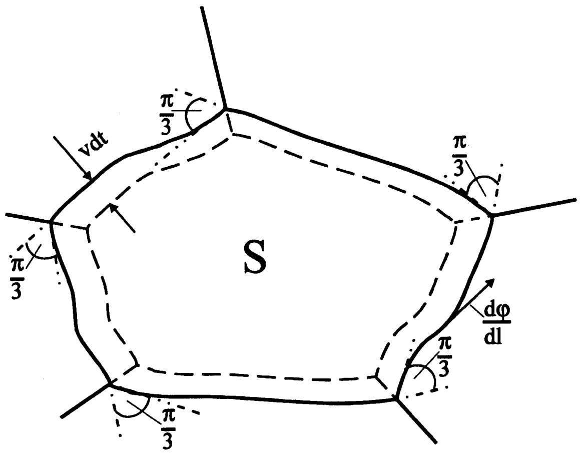

Fig. 1. Definition of parameters for the effect of triple junctions for a calculation of the rate of grain area change.

the following we consider a system of three grain boundaries with a common triple junction as depicted in Fig. 2. Two of the boundaries are curved, which results in a force on the entire boundary-junction-system. The convex shape of the boundaries corresponds to the curvature of the grains with less than six sides in a polycrystal. Hence, this geometry is representative for grain with $n<6$, where n is the number of sides of a grain in 2D.

During steady state motion of the whole system the velocity V parallel to the x-axis (Eq. (2)) is related to the normal displacement rate v

$$v = V\cos\varphi = V\frac{y'}{(1+(y')^2)^{1/2}} \tag{6}$$

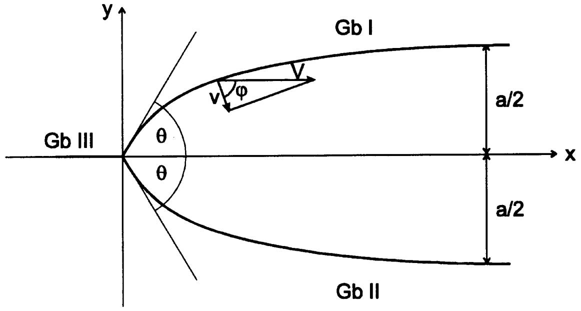

Fig. 2. Configuration of grain boundaries at a triple junction during steady state motion for n=6.

where $y(x)$ is the shape of the upper part of the curved boundary [6]. (Due to the mirror symmetry of the problem relative to the x-axis, the shape of the lower boundary is the negative equivalent).

From Eqs (2), (6) and taking into account the expression for the curvature K

$$K = -\frac{y''}{(1+(y')^2)^{3/2}} \tag{7}$$

we obtain the equation for the shape of the moving grain boundary

$$y'' = -\frac{v}{m_b\sigma}y'(1+(y')^2) \tag{8}$$

With the boundary conditions $y(0)=0$, $y(\infty)=a/2$, $y'(0)=\tan\Theta$, Eq. (8) has the solution

$$y(x) = \xi\arccos(e^{-x/\xi+c_1}) + c_2 \tag{9}$$

where $\xi = a/2\Theta$, $c_1 = \ln(\sin\Theta)$, $c_2 = -\xi(\pi/2-\Theta)$.

The meaning of the length a and the angle Θ is clear from Fig. 2. A driving force $\sigma(2\cos\Theta-1)$ acts on the triple junction from the curved boundaries. Introducing the mobility of the triple junction m_{tj}, its velocity reads

$$V_{tj} = m_{tj}\sigma(2\cos\Theta-1) \tag{10}$$

Due to the fact that the driving force acting on the grain boundary is a 2D pressure (force/length) and the driving force on the triple junction is a force, the dimensions of grain boundary and triple junction mobility are different, so that their ratio m_b/m_{tj} has the dimension of a length.

The velocity V of steady state motion of the system is

$$V = \frac{2\Theta m_b\sigma}{a} \tag{11}$$

and the steady state value for the angle Θ can be found from the equation

$$\frac{2\Theta}{2\cos\Theta-1} = \frac{m_{tj}a}{m_b} = \Lambda \tag{12}$$

If a triple junction is perfectly mobile and does not drag grain boundary motion, then $\Lambda \to \infty$ and $\Theta \to \pi/3$, i.e. the equilibrium angle at a triple junction in the uniform grain boundary model. In contrast, however, if the mobility of the triple junction is relatively low (strictly speaking, if $m_{tj}a \ll m_b$ then $\Theta \to 0$ (Fig. 3 [6]). It is particularly emphasized that the angle Θ is completely defined by the dimensionless parameter Λ, which, in turn, is a function of not only the ratio of triple junction and grain boundary mobility, but of the grain size as well. Thus, the term "triple junction of low mobility" is equivalent to a "small value of Λ".

Experimental investigations carried out with the shape of the grain boundary system shown in Fig. 2 revealed that triple junctions do possess a finite mobility [7,8,11]. In particular, it was demonstrated that the vertex angle Θ at the triple junction can deviate distinctly from the equilibrium value, when a low mobility of the triple junction hinders the motion of the grain boundaries. In fact, a transition from triple junction kinetics to grain boundary kinetics was observed (Fig. 3) [7].

3.2. *Vertex angle for* $\boldsymbol{n}>6$

The model behavior of grains with topological class $n>6$ can be considered by the steady state motion of a grain boundary system shown in Fig. 4. Again, we assume uniform grain boundary properties and quasi-two-dimensionality. The steady state motion of this system is determined by

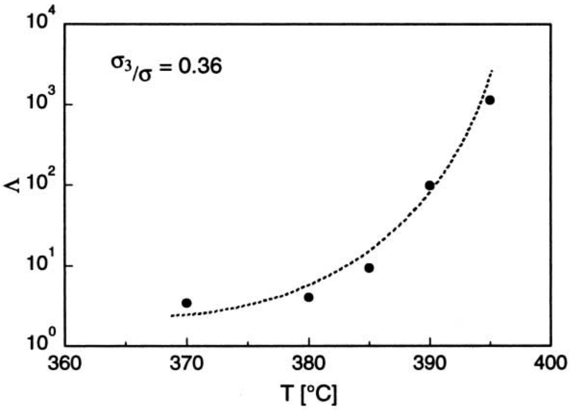

Fig. 3. Measured temperature dependence of the criterion Λ for Zn tricrystals.

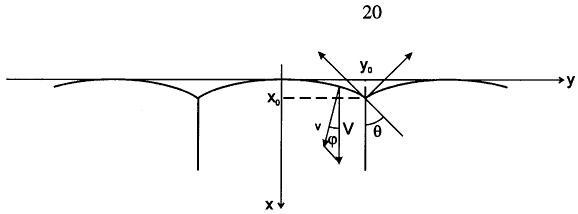

Fig. 4. Configuration of grain boundaries at triple junctions during steady state motion for $n>6$.

the set of Eqs. (2, 6–8) only with different boundary and initial conditions: $y'(0)=\infty$, $y'(x_0)=\tan\Theta$, $y(0)=0$ to yield

$$y(x) = -\frac{x_0}{\ln\sin\Theta}\arccos(e^{(x/x_0)\ln\sin\Theta}) \tag{13}$$

The velocity of the triple junction can be expressed as (Fig. 4)

$$V_{tj} = m_{tj}\sigma(1-2\cos\Theta) \tag{14}$$

The velocity of steady state motion of the boundary system is

$$V = -\frac{m_b\sigma}{x_0}\ln\sin\Theta \tag{15}$$

The length x_0 replaces the role of the grain size a in the previous case (Fig. 4).

From Eq. (14) and Eq. (15) we obtain Λ, which describes the influence of the triple junction mobility on grain boundary migration

$$-\frac{\ln\sin\Theta}{1-2\cos\Theta} = \frac{m_{tj}x_0}{m_b} = \Lambda \tag{16}$$

Obviously, for $\Lambda \gg 1$, when the boundary mobility determines the kinetics of the system the angle Θ tends to its equilibrium value ($\pi/3$).

Again, the angle Θ changes when a low mobility of the triple junction starts to drag the motion of the boundary system. However, as can be seen from Eq. (16) and Fig. 3, in this case the steady state value of the angle Θ *increases* as compared to the equilibrium state.

3.3. Effect on Von Neumann–Mullins relation

Let us consider how the Von Neumann–Mullins relation Eq. (5) looks in the light of the mentioned results.

It was pointed out that the derivation of the Von Neumann–Mullins relation is based on three assumptions. One of them is the requirement imposed on the triple junction, namely, the mobility of triple junctions is infinitely large; therefore, the contact angles at triple junctions are in equilibrium and for a system of uniform grain boundaries the angles are 120°. The reported evidence of a finite mobility of triple junctions and the marked deviation of the vertex angle Θ from the equilibrium value requires reconsideration of the influence of triple junction drag on the Von Neumann–Mullins relation.

For this we assume that the influence of the triple junctions is rather large, but nevertheless, the motion of the system can be viewed as grain boundary motion, since the driving force is still due to grain boundary curvature, i.e. the role of the triple junctions is reduced to a change of the angle Θ. As mentioned above Eq. (12) describes the steady state value of the angle Θ. Of course, triple junctions in real polycrystals rarely experience steady state motion. However, the attainment of a true steady state is not important in this context. Even if the angle Θ is not in steady state with the moving triple junction, it will be different from the equilibrium angle $\Theta = \pi/3$ as assumed for the Von Neumann–Mullins relation and thus, will affect the kinetics with the same tendency as in steady state.

Let us consider the motion of a boundary driven by grain boundary curvature with a triple junction. Due to the fact that triple junctions have their own mobility the motion of such a boundary can be considered as a motion of a boundary with mobile defects [13]. The velocity of such a boundary is given by

$$V = P_{\mathrm{eff}} \cdot m_{\mathrm{b}} \tag{17}$$

where P_{eff} is the effective driving force.

$$P_{\mathrm{eff}} = \sigma K - \frac{f}{a} \tag{18}$$

Here a is the spacing of junctions, f is the dragging force of a junction with the Einstein relation

$$f = \frac{V}{m_{\mathrm{tj}}} \tag{19}$$

we arrive at

$$V\left(1 + \frac{m_{\mathrm{b}}}{m_{\mathrm{tj}} a}\right) = m_{\mathrm{b}} \sigma K \tag{20}$$

From equations (12), (16), (17) and (20)

$$V = \frac{m_{\mathrm{b}} \sigma K}{1 + \frac{1}{\Lambda}} \tag{21}$$

In our consideration the contact angle Θ is assumed to be close to the equilibrium angle, so the criterion Λ is large. That is why the rate of area change can be expressed as

$$\frac{\mathrm{d}S}{\mathrm{d}t} = -m_{\mathrm{b}} \sigma \oint \frac{\mathrm{d}\varphi}{1 + \frac{1}{\Lambda}} = -\frac{A_{\mathrm{b}}}{1 + \frac{1}{\Lambda}} \oint \mathrm{d}\varphi \tag{22}$$

Because the integral $\oint \mathrm{d}\varphi$ for n-sided grain under the impact of a non-equilibrium contact angle is equal to [9]

$$\oint \mathrm{d}\varphi = 2\pi - n(\pi - 2\theta)$$

the Eq. (22) takes the form

$$\frac{\mathrm{d}S}{\mathrm{d}t} = -\frac{A_{\mathrm{b}}}{1 + \frac{1}{\Lambda}} [2\pi - n(\pi - 2\theta)] \tag{23}$$

For grains with $n < 6$ Eq. (23) reads

$$\frac{\mathrm{d}S}{\mathrm{d}t} = -\frac{A_{\mathrm{b}}}{1 + \frac{2\cos\theta - 1}{2\theta}} [2\pi - n(\pi - 2\theta)] \tag{24}$$

Since the limited mobility of triple junctions reduces the steady state value of the angle Θ as compared to the equilibrium angle, the shrinking rate of grains with $n < 6$ decreases. In other words, the influence of the triple junction decreases the vanishing rate of grains with small topological classes.

Correspondingly, for grains with $n>6$ with equations (16) and (23) we arrive at

$$\frac{dS}{dt}=\frac{A_b[n(\pi-2\theta)-2\pi]}{1-\frac{1-2\cos\theta}{\ln(\sin\theta)}} \qquad (25)$$

In this case the dragging influence of triple junctions increases the angle Θ and also slows down the process of grain structure evolution. In other words, microstructural evolution proceeds more slowly due to triple junction drag for any n-sided grain. Since the actual magnitude of Θ is determined by triple junction and grain boundary mobility as well as the grain size there is no unique dividing line between vanishing and growing grains with respect to their topological class anymore.

4. Grain boundary motion controlled by triple junction kinetics

4.1. Steady state grain boundary shape

In the following we consider the rate of change of a grain area S when the motion of grain boundaries is controlled by the motion (mobility) of triple junctions. This is different from the case where boundary motion is only dragged by a small triple junction mobility. To begin with we will show that in the course of grain growth in 2D systems under triple junction control the grains will eventually be bordered by straight lines, i.e. they will assume a polygonal shape.

Let us consider the curvature of a grain boundary system with triple junctions (Figs 2 and 4). The expression for the curvature K can be found from equations (7), (9)–(12), (13). For the system shown in Fig. 2 we obtain with $\xi=a/2\Theta$

$$K=\frac{1}{\xi}e^{-x/\xi+\ln\sin\Theta}=\frac{2\Theta}{a}e^{-(2\Theta/a)x}\sin\Theta \qquad (26)$$
$$=\frac{\Lambda}{a}\sin\Theta(2\cos\Theta-1)e^{-(2\Theta/a)x}$$

while for the system shown in Fig. 4

$$K=\frac{\ln\sin\Theta}{x_0}e^{(x/x_0)\ln\sin\Theta}=\frac{\Lambda}{x_0}(1-2\cos\Theta)e^{(x/x_0)\ln\sin\Theta} \qquad (26a)$$

In either case, the grain boundary curvature K approaches zero, since for triple junction kinetics $\Lambda\rightarrow 0$, i.e. the grain structure of 2D polycrystals essentially comprises straight grain boundaries which extend between the triple junctions. In other words, the granular arrangement in a 2D polycrystal is represented by a system of polygons. Owing to the imbalance of surface tensions at each junction, the polygonal structure is liable to change with time, i.e. to coarsen (Section 3.3). In this context it is interesting whether the structure can assume a stable arrangement that would freeze grain growth. For boundary mobility controlled grain growth like in the Von Neumann–Mullins case (Eq. (5)), but equally in the instance of junction drag (Eq. (23)), grain growth would cease if all grains assume a hexagonal shape (n=6, Θ=60°) even though this would not be the lowest free energy state of the crystal.

The case of junction mobility controlled grain growth requires a different topology for grain growth stagnation, i.e., all grains would have to assume the shape of a regular polygon, irrespective of their number of sides, except for a triangle. As shown in Appendix A, a grain with a shape of a regular polygon remains stable, i.e., does not undergo a shape change except for a triangular shape. Correspondingly, a 2D arrangement of grains with regular polygonal shape would “freeze”, except if it contains triangular grains. The hexagonal structure belongs to this set of stable geometries only, if it were equilateral. On the other hand, any other space filling arrangement of regular polygon is a potential stable structure, if it can be attained.[1] The only exception is a triangle, and any arrangement of regular polygons which con-

[1] It is not known to the authors whether space filling topological arrangements of regular polygons exist besides regular hexagons.

tains at least a single triangle would also be observed to behave unstably.

We reason that this phenomenon has important consequences for the development of grain growth. Let us take a look at the evolution of a shrinking grain in the course of grain growth. The topological class of such a grain should be smaller than 6, naturally taking into account all corrections to the Von Neumann–Mullins relation, given in Section 3. As shown above the transition between boundary and triple junction kinetics does not only depend on grain boundary and triple junction mobility, but on the size of a grain as well. When the size of a grain progressively diminishes there comes a time when boundary kinetics becomes replaced by junction kinetics. This will happen to grains of the topological class n=4 or n=5 which are bound to shrink even after such a transition to triple junction kinetics. Grains of topological class n=3 will collapse without transforming into a regular polygon. Since the kinetics of triple junctions are significantly slower than the boundary kinetics, the four- and five-sided polygons will shrink, and eventually contract to a point although at a markedly smaller rate. Experimentally this phenomenon will manifest itself in the mean value of the topological class of vanishing grains. In Fig. 5 experimental data of grain growth in aluminum foil with 2D (columnar) structure is presented, in terms of the grain size dependence of the mean topological class <n> [14]. Extrapolation of this experimental dependence to zero area yields the mean value of the topological class of vanishing grains. As can be seen <n>(0)≅4.2, i.e. n=4 is the smallest topological class to shrink in a stable manner.

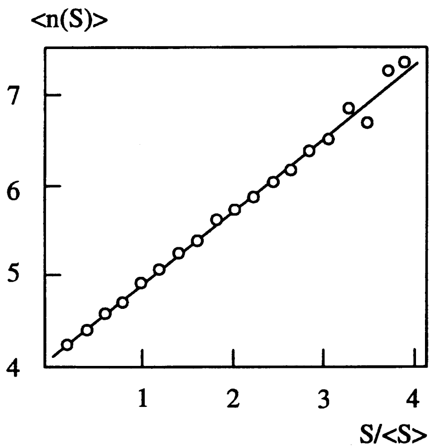

Fig. 5. Dependence of the mean topological class <n(s)> on "grain size" s/<s> (normalized by the average grain size) for pure Al [13].

4.2. Kinetics of structure evolution

Let us finally consider the behaviour of an n-sided polygon (Fig. A1). The rate of change of its area S can be represented as

$$\frac{dS}{dt} = \oint V\, d\ell = -V_n \oint d\ell = -V_n P \tag{27}$$

where V_n is the boundary velocity parallel to the boundary normal, P is the perimeter of the polygon.

As can be seen from Fig. A1

$$\begin{aligned} V_n &= V_{tj} \cdot \cos(\pi/2-\Theta) \\ &= m_{tj} \cdot \sigma[2\cos\Theta-1]\cos(\pi/2-\Theta) \end{aligned} \tag{28}$$

Since the angle Θ for a regular n-sided polygon is equal to $\pi(n-2)/2n$, Eq. (28) can be rewritten as

$$V_n = m_{tj} \cdot \sigma[2\sin(\pi/n)-1]\cos(\pi/n) \tag{29}$$

where n is the topological class of the grain. From equations (27) and (29) we obtain the rate of change of the grain area S, when grain boundary motion is controlled by the displacement of the triple junctions

$$\frac{dS}{dt} = -m_{tj}\sigma[2\sin(\pi/n)-1]\cos(\pi/n)P \tag{30}$$

4.3. Effect on microstructure evolution

In essence, therefore, a limited triple junction mobility always slows down the evolution of grain microstructure of polycrystals, irrespective whether the topological class of the considered grain is smaller or larger than 6. The mere fact that there is a growing grain with triple junctions of low mobility requires the existence of other grains with n<6 to surround it. There is no point in discussing to which grain their common junction belongs. The only exception holds for n=6, since a hexagonal grain structure becomes unstable when the contact angle $2\Theta \neq 2\pi/3$. Since the actual magnitude of Θ is determined by the triple junction and grain boundary mobility as well as the grain size and is independent of the number of sides of a grain, there is no unique dividing line between vanishing and growing grains with respect to their topological class anymore, like n=6 in the Von Neumann–Mullins approach.

When grain boundary migration is completely controlled by triple junction motion, it is interesting to compare the obtained Eq. (30) with the Von Neumann–Mullins relation Eq. (5), which gives the rate of area change of a grain with topological class n under the condition that the triple junctions do not affect grain boundary motion [2]. Evidently, the qualitative behaviour of equations (4) and (5) is similar. Grains with $n>6$ will grow while those with $n<6$ will disappear in accordance with both equations (5) and (30). What distinguishes equations (30) and (5) is, firstly, the dependence of the rate of change on the topological class n. According to Eq. (5), dS/dt increases infinitely with the number n, whereas for the triple junction kinetics

$$\lim_{n\to\infty}\frac{dS}{dt} = m_{tj}P\sigma$$

The second distinctive difference is connected with the dependence of the rate of area change on the grain size. The Von Neumann–Mullins relation Eq. (5) does not depend on the grain size, whereas Eq. (30) relates the rate of area change to the grain size through the perimeter P of the grain.

5. Conclusions

The effect of triple junction mobility on the rate of change of the grain area during 2D grain growth was investigated. It was found that a finite junction mobility exerts a drag on the adjoining grain boundaries. This is reflected by a deviation of the grain vertex angles at triple junctions from their equilibrium value $2\pi/3$ and correspondingly, by a modification of the Von Neumann–Mullins relation. It was shown that for the situation when the triple junction influence on grain boundary motion is large enough, but nevertheless the grain boundary motion is controlled by grain boundary kinetics, the triple junction influence results in a reduced rate of microstructure evolution during grain growth, since the effective topological class of growing grains ($n>6$) is decreased and of shrinking grains ($n<6$) is increased. The considered problem and thus, the obtained relations, are relevant for the kinetics of microstructure evolution in polycrystals, especially in nanocrystalline systems, and in the case of abnormal grain growth.

It was shown that for triple junction kinetics, i.e. when grain boundary motion is controlled by the displacement rate of triple junctions, the Von Neumann–Mullins relation is replaced by a relation, that does not only take into account the topological class of a grain but its perimeter as well. Moreover, the structure would stabilize if it attains an arrangement of regular polygons, in contrast to a hexagonal arrangement that would frustrate a structure in the regime of boundary mobility controlled grain growth, e.g. in the Von Neumann–Mullins case.

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Appendix A

Let us consider a regular n-sided polygon, where one part, which includes 2 sides and 3 angles, is slightly different from the other, regular part of a polygon (Fig. A1). The angle α is the angle between the bisector of the angle ψ and the basis of the triangle considered; γ is the angle of a regular n-sided polygon, $\gamma=(\pi/n)(n-2)$. According to

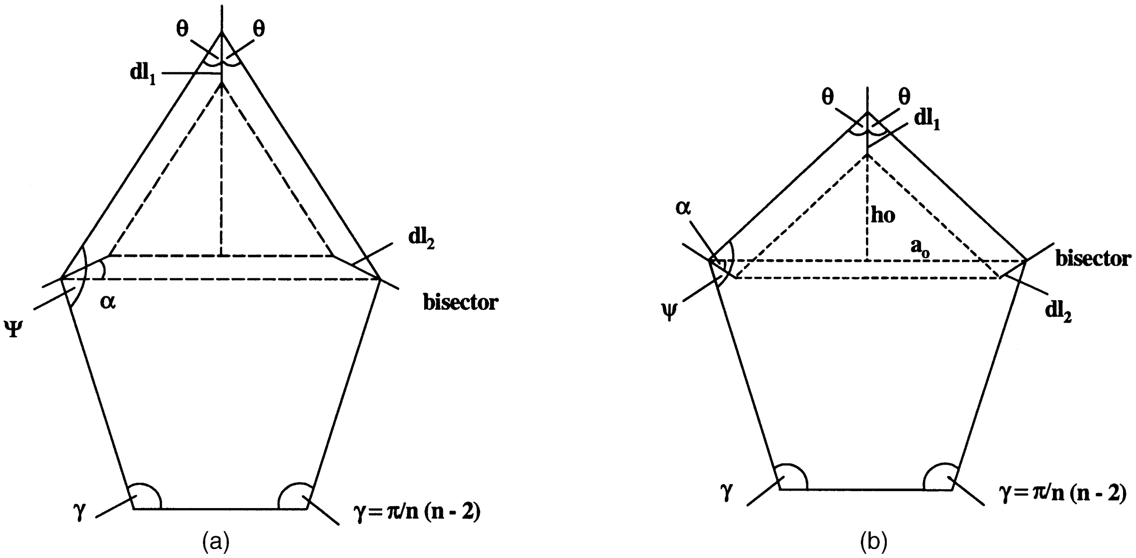

Fig. A1. Sketch of the shape evolution of an *n*-sided polygon for two alternative directions of the bisector.

the considered conditions there are three "non-regular" angles: one of them is equal to 2Θ (Fig. A1), two others are equal to ψ. Obviously, $2\Theta+2\psi=3\gamma$, or $\psi=(3\gamma-2\Theta)/2$.

The change of the angle Θ due to a displacement of the triple junction can be expressed as

$$\tan(\Theta+\mathrm{d}\Theta)\cong\tan\theta+(1+\tan^2\Theta)\mathrm{d}\Theta \qquad \text{(A1)}$$

or

$$(1+\tan^2\Theta)\mathrm{d}\Theta=\frac{a_0-\mathrm{d}l_2\cdot\cos\alpha}{h_0-\mathrm{d}l_1-\mathrm{d}l_2\sin\alpha}-\tan\Theta \qquad \text{(A2)}$$

The displacements of the triple junctions during the time interval *dt* can be written as [6,9]

$$\mathrm{d}l_1=V_1\mathrm{d}t=m_{\mathrm{tj}}\sigma(2\cos\Theta-1)\mathrm{d}t \qquad \text{(A3)}$$

$$\mathrm{d}l_2=V_2\mathrm{d}t=m_{\mathrm{tj}}\alpha\left(2\cos\frac{\psi}{2}-1\right)\mathrm{d}t$$

and the change of the angle Θ can be expressed as

$$(1+\tan^2\Theta)\mathrm{d}\Theta=\frac{a_0-m_{\mathrm{tj}}\sigma\left(2\cos\frac{\psi}{2}-1\right)\cos\left[\frac{\pi}{2}-\left(\Theta+\frac{\psi}{2}\right)\right]}{h_0-m_{\mathrm{tj}}\sigma(2\cos\Theta-1)\mathrm{d}t-m_{\mathrm{tj}}\sigma\left(2\cos\frac{\psi}{2}-1\right)\sin\left[\frac{\pi}{2}-\left(\Theta+\frac{\psi}{2}\right)\right]\mathrm{d}t}-\frac{a_0}{h_0}$$
$$=\frac{m_{\mathrm{tj}}\sigma a_0\mathrm{d}t}{h_0^2}\left[-\left(2\cos\frac{\psi}{2}-1\right)\sin\left(\Theta+\frac{\psi}{2}\right)\mathrm{ctn}\,\Theta+2\cos\Theta-1+\left(2\cos\frac{\psi}{2}-1\right)\cos\left(\frac{\psi}{2}+\Theta\right)\right] \qquad \text{(A4)}$$

The rate of a change of the angle Θ reads

$$\frac{\mathrm{d}\Theta}{\mathrm{d}t}=\frac{m_{\mathrm{tj}}\sigma a_0}{h_0^2}\cos^2\Theta\left[-\left(2\cos\frac{\psi}{2}-1\right)\sin\left(\Theta+\frac{\psi}{2}\right)\mathrm{ctn}\Theta+2\cos\Theta-1+\left(2\cos\frac{\psi}{2}-1\right)\cos\left(\frac{\psi}{2}+\Theta\right)\right] \qquad \text{(A4a)}$$

For $\Theta=\gamma/2$ we arrive at

$$\frac{d\Theta}{dt} = \frac{m_{tj}\sigma a_0}{h_0^2}\cos^2\frac{\gamma}{2}\left[-\left(2\cos\frac{\gamma}{2}-1\right)\sin\gamma\,\mathrm{ctn}\frac{\gamma}{2} + \left(2\cos\frac{\gamma}{2}-1\right) + \left(2\cos\frac{\gamma}{2}-1\right)\cos\gamma\right] = 0 \quad (A5)$$

For the case of an alternative direction of the bisector (Fig. A1(b)) we obtain the same equation. Actually, for this configuration

$$\alpha = \frac{\psi}{2}-\left(\frac{\pi}{2}-\Theta\right)$$

$$2\psi + 2\Theta = 3\gamma$$

and, as can be seen

$$\frac{d\Theta}{dt} = \frac{m_{tj}\sigma a_0}{h_0^2}\cos^2\Theta\left[-\left(2\cos\frac{\psi}{2}-1\right)\cos\alpha\,\mathrm{ctn}\,\Theta + (2\cos\Theta-1)-\left(2\cos\frac{\psi}{2}-1\right)\sin\alpha\right]$$

We arrive at the same equation, which for $\Theta=(\gamma/2)$ gives the same result, namely

$$\frac{d\Theta}{dt}\Big|_{\Theta=\frac{\gamma}{2}} = 0 \quad (A6)$$

Consequently, we derived a general expression, which shows that for n-sided polygons at $\Theta\rightarrow(\gamma/2)$ the rate of change of the angle Θ, $(d\Theta/dt)\rightarrow 0$, where γ is the angle for a regular n-sided polygon.

The next steps are to prove that the equilateral shape is stable, in other words that the system — a regular n-sided polygon — returns to the equilateral state after being displaced from this state. The sign of the derivative $(d/d\Theta)(d\Theta/dt) = \eta(\Theta,n)|_{\Theta(\gamma/2)}$ is an index of the stability of the equilateral shape, namely this shape will be stable if the function $\eta(\Theta,n)$ is negative at the point $\Theta=(\gamma/2)$. Actually, if the function $\eta(\Theta,n)$ is positive at $\Theta=(\gamma/2)$ the system will move in the direction prescribed by the sign of the deviation $d\Theta$: $d(d\Theta/dt)=\eta(\Theta,n)|_{\Theta(\gamma/2)}d\Theta$, while the stable behavior of the system is characterized by the opposite reaction to the perturbation. Namely, if a deviation $d\Theta$ from the position $\Theta=(\gamma/2)$ is positive, the system will return to its stable position by decreasing the angle Θ. Similarly, if a deviation $d\Theta$ is negative, a stable system will respond by increasing Θ to return to equilibrium. Consequently, only a negative value of the function $\eta(\Theta,n)$ reflects a stable behavior of the system.

The desired function $\eta(\Theta,n)$ can be easily derived from Eq. (A5)

$$\eta(\Theta,n)|_{\Theta=\frac{\gamma}{2}} = \frac{d}{d\Theta}\left(\frac{d\Theta}{dt}\right)\Big|_{\Theta=\frac{\gamma}{2}} = \frac{m_{tj}\sigma a_0}{h_0^2}\frac{d}{d\Theta}\left\{\cos^2\Theta\left[2\cos\left(\frac{3}{4}\gamma-\frac{\Theta}{2}\right)-1\right]\left[\cos\left(\frac{3}{4}\gamma+\frac{\Theta}{2}\right)-\sin\left(\frac{3}{4}\gamma+\frac{\Theta}{2}\right)\mathrm{ctn}\,\Theta\right] + (2\cos\Theta-1)\right\}\Big|_{\Theta=\frac{\gamma}{2}} \quad (A7)$$

$$\frac{m_{tj}\sigma a_0}{h_0^2}\frac{d}{d\Theta}(\cos^2\Theta)\left[\left[2\cos\left(\frac{3}{4}\gamma-\frac{\Theta}{2}\right)-1\right]\left[\cos\left(\frac{3}{4}\gamma+\frac{\Theta}{2}\right)-\sin\left(\frac{3}{4}\gamma+\frac{\Theta}{2}\right)\mathrm{ctn}\,\Theta\right] + 2\cos\Theta-1\right]\Big|_{\Theta=\frac{\gamma}{2}} + \frac{m_{tj}\sigma a_0}{h_0^2}\cos^2\Theta\cdot\frac{d}{d\Theta}\left[\left[2\cos\left(\frac{3}{4}\gamma-\frac{\Theta}{2}\right)-1\right]\left[\cos\left(\frac{3}{4}\gamma+\frac{\Theta}{2}\right)-\sin\left(\frac{3}{4}\gamma+\frac{\Theta}{2}\right)\mathrm{ctn}\,\Theta\right] + (2\cos\Theta-1)\right]\Big|_{\Theta=\left(\frac{\gamma}{2}\right)} \quad (A8)$$

As shown above, the first term on the right-hand side is equal to zero at $\Theta=(\gamma/2)$. So, the function $\eta(\Theta,n)|_{\Theta(\gamma/2)}$ can be represented as

$$\eta(\Theta,n)|_{\Theta=\frac{\gamma}{2}} = \frac{m_{tj}\sigma a_0}{h_0}\cos^2\frac{\gamma}{2}\left\{\sin\frac{\gamma}{2}\left(\cos\gamma-\sin\gamma\,\mathrm{ctn}\frac{\gamma}{2}\right) + \left(2\cos\frac{\gamma}{2}-1\right)\left(\frac{\sin\gamma}{\sin^2\frac{\gamma}{2}}-\frac{1}{2}\sin\gamma-\frac{1}{2}\cos\gamma\,\mathrm{ctn}\frac{\gamma}{2}\right)--2\sin\frac{\gamma}{2}\right\} \equiv \equiv B\left(\cos^2\frac{\gamma}{2}\right)\eta_0(\gamma) \quad (A9)$$

Table A1
Value of the function $\eta(\Theta,n)|_{\Theta(\gamma/2)}$ for n-sided polygons

n	$\eta(\Theta,n)|_{\Theta=\frac{\gamma}{2}} = B\left(\cos^2\frac{\gamma}{2}\right)\eta_0(n)$ in terms of B
3	+0.30
4	−0.75
5	−0.77
6	−0.62
7	−0.52
8	−0.42
9	−0.35
10	−0.29
11	−0.24
12	−0.20
–	–
18	−0.0975

where $\eta_0(\gamma)$ is defined by this equation.

Inasmuch as the angle γ is defined by the topological class n of regular polygons, namely, $\gamma=(\pi/n)(n-2)$, the magnitude and, what is more important, the sign of the function η can be easily determined (Table A1). If in contrast to the assumption made above the polygon is not symmetrical, then it will be symmetrized during grain boundary motion. For example, consider an n-sided polygonal grain (Fig. A1), for which one of the triple junctions, e.g. triple junction 1, deviates from the position of a bisector of Θ by $d\Theta$. The change of $\tan(\Theta + d\Theta)$ in a time interval dt is again described by Eq. (A3). Hence, the stability obtained for $\Theta\to\gamma/2$ requires an equilateral shape of the polygon. In summary, the steady state shape of a 2D grain under triple junction kinetics is an equilateral polygon.

As can be seen, an equilateral shape is stable indeed for all polygons. The sole exception is a triangle.

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