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A novel concept to determine the mobility of grain boundary quadruple junctions

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Abstract

We put forward a new concept which makes it possible to study experimentally the mobility of a grain boundary quadruple point.

Keywords: Grain boundaries; Quadruple junctions; Mobility; Grain boundary motion

1. Introduction

Traditional textbook knowledge of grain growth in polycrystals is based on the concept of curvature driven grain boundary motion. The other structural elements of connected grain boundaries are considered only as incidental geometrical components of the boundaries in a polycrystal.

However, several recent theoretical and experimental studies provide evidence that triple junctions do affect boundary motion, because the kinetics of triple junctions may be different from the kinetics of the adjoining grain boundaries. This has serious consequences for microstructure evolution during grain growth [1–3].

Besides grain boundaries and triple junctions there is only one more topological element of a 3D arrangement of connected boundaries, a grain boundary quadruple point at the location where four grains meet. At the same time this point is the location where four grain boundary triple lines intersect (Fig. 1). The latter definition lends itself to the study of quadruple point motion.

1.1. Theory of steady state quadruple junction motion

Every triple junction is the geometrical location of points which belong to three grains. The shape of the triple junction line in our model (Fig. 2) resembles the shape of a grain boundary in a tricrystal comprising a model grain boundary system with a triple junction: far from the quadruple point all three boundaries are rectilinear and parallel each to other.

In such a configuration motion proceeds under the action of the triple junction line tension γ^1. We will consider this problem in the framework of a uniform triple junction model, i.e. all triple lines possess equal line tensions and mobilities irrespective of the misorientation of the adjacent grains and the crystallographic orientation of the boundaries, also the mobility of a triple junction is assumed to be independent of its velocity.

The given assumptions require symmetry with respect to any plane that contains the curved triple line (Fig. 1). The equation of motion for each element of a triple line, i.e. the velocity of the triple junction defines the differential equation of the shape $y(x)$ of a moving triple junction. Actually, the velocity of a normal motion of a triple junction element is

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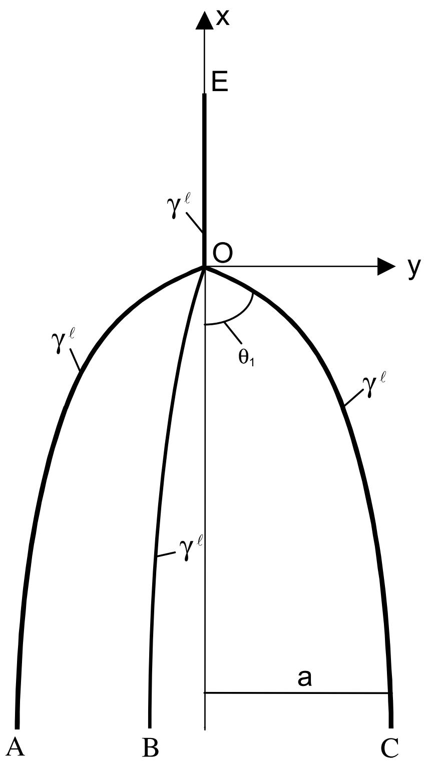

Fig. 1. Four grain arrangements with four triple lines (OA, OB, OC, OE) and one quadruple point at O. The angle θ_1 is the vertex angle of a triple line at the quadruple junction, a is the (half) dimension of the grain bounded by the OA, OB and OC.

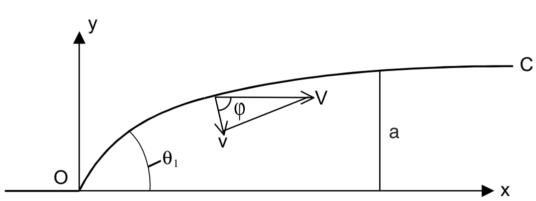

Fig. 2. Cross-section parallel to the a grain boundary triple line OC in Fig. 1.

$$v = m_{tj}\gamma^{l}\kappa \tag{1a}$$

where

$$\kappa = -y'' \cdot [1 + (y')^2]^{-3/2} \tag{1b}$$

is the curvature of the triple line element. Because during steady-state motion the velocity V is constant (Fig. 2).

$$v = V\cos\theta_1 = Vy'[1 + (y')^2]^{-1/2} \tag{2}$$

One can solve Eq. (1)

$$y'' = -\frac{V}{m_{tj}\gamma^{l}}y'[1 + (y')^2] \tag{3}$$

under the boundary conditions

$$y(0) = 0$$

$$y(\infty) = a/2$$

$$y'(0) = \tan\theta_1$$

where m_{tj} is the mobility of the triple junction, γ^{l} is the line tension of the triple junction, $y(x)$ is the shape of the triple line, θ_1 is the angle at the tip of the triple junctions at the quadruple point (see Fig. 1).

For derivation of the force P acting on the quadruple point, let us consider a plane that contains the triple line OC and the x-axis in Fig. 1. The components of all triple line tensions acting on the quadruple junction in this plane is $P = 2\gamma^{l}\cos 60^\circ \cdot \cos\theta_1 + \gamma^{l}\cos\theta_1 - \gamma^{l}$. Then, the velocity of the quadruple point motion reads

$$\begin{aligned} V_{qp} &= m_{qp}[2\gamma^{l}\cos 60^\circ \cdot \cos\theta_1 + \gamma^{l} \cdot \cos\theta_1 - \gamma^{l}] \\ &= m_{qp}\gamma^{l}[2\cos 60^\circ \cdot \cos\theta_1 + \cdot \cos\theta_1 - 1] \end{aligned} \tag{4}$$

where m_{qp} is the mobility of the quadruple point.

Eqs. (3) and (4) define the problem comprehensively. Integration of Eq. (3) yields the shape of a steady-state moving triple junction system with a quadruple point.

$$\begin{aligned} y(x) &= \varsigma \arccos(e^{-x/\varsigma + C_1}) + C_2 \\ \varsigma &= \frac{a}{2\theta_1} \\ C_1 &= \frac{1}{2}\ln(\sin\theta_1)^2 \\ C_2 &= \varsigma(\pi/2 - \theta_1) \end{aligned} \tag{5}$$

Evidently, a steady-state motion of the grain boundary system with a quadruple point is possible indeed.

The velocity V of steady-state motion of the triple junction system is equal to

$$V = \frac{2\theta_1 m_{tj}\gamma^{l}}{a} \tag{6}$$

From the equations for triple junction and quadruple point motion (Eqs. (3) and (4)) we derive the steady-state value of the angle θ_1

$$\begin{aligned} \Lambda_{qp} &= \frac{m_{qp}a}{m_{tj}} = \frac{2\theta_1}{\cos\theta_1(2\cos 60^\circ + 1) - 1} \\ &= \frac{2\theta_1}{2\cos\theta_1 - 1} \end{aligned} \tag{7}$$

If a quadruple point is perfectly mobile and does not drag grain boundary motion, then $\Lambda_{qp} \to \infty$ and $\theta_1 \to \pi/3$, which is the equilibrium angle between quadruple point and triple junction line in the uniform boundary and triple line model. In contrast, however, if the mobility of the quadruple point is relatively low (strictly speaking, if $m_{qp}a \ll m_{tj}$) then $\theta_1 \to 0$. The angle θ_1 is unambiguously defined by the dimensionless parameter Λ_{qp}, which, in turn, is a function of not only the ratio of quadruple point and triple junction mobility, but of the grain size as well.

It is important to realize that we consider the steady-state motion in our four grain-system. By this is meant that also triple junction motion and grain boundary motion proceed in steady state. This is indeed warranted. To prove this let us consider an arbitrary section through the four grain system which contains the y-axis. This plane will intersect with at least two of the three grain boundaries below the quadruple junction, for instance along OB′ and OC′ in Fig. 3. The lines of intersection form a standard steady state 2D boundary configuration with a triple junction (Fig. 4). The vertex angle θ at the point O is determined by the interaction of the grain boundary surface tensions at this point and the quadruple junction.

In contrast to standard steady state triple junction configuration the boundaries, however, do not run straight in a plane perpendicular to the section plane, rather they are curved. This is depicted in Fig. 5 where the intersection of the four grains with a plane perpendicular to the y-axis—containing the points D, D′, D″ in Fig. 3—is shown. The configuration comprises of a triangle with convex boundaries. This configuration is bound to move inward even far from the quadruple junction. To be able to observe a steady state motion of the quadruple junction the shrinkage of this convex triangle has to be slow compared to the motion of the quadruple junction.

The motion of a quadruple point is a true 3D problem and cannot be reduced to a quasi 2D configuration like for triple junctions. Therefore, experimental observation of quadruple point motion will require 3D imaging techniques. Respective facilities have recently become available [4]. We anticipate that advanced X-ray tomography with synchrotron radiation can soon be utilized to reveal the temporal development of a four grain arrangement with quadruple junction.

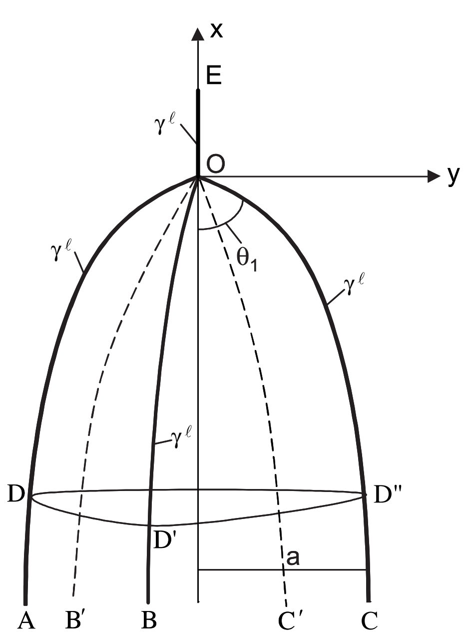

Fig. 3. Sections through the four grain systems: DD′D″ denotes a plane perpendicular to the y-axis that intersects all four grains (see Fig. 5).

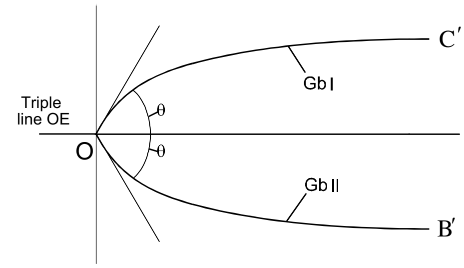

Fig. 4. Arbitrary section along the y-axis. The plane intersects two grain boundaries of the grain inside along OB′ and OC′ in Fig. 3.

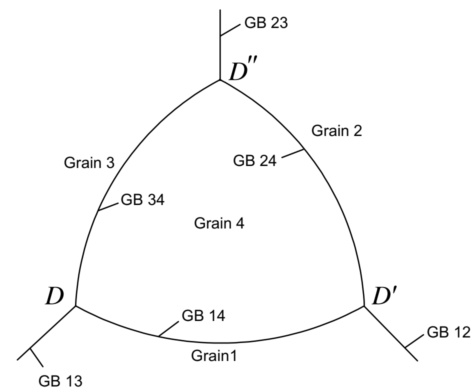

Fig. 5. Cross-section through the four grain arrangements shown in Fig. 3. The lines DD′, D′D″ and D″D denote the grain boundaries between the three exterior grains and the interior grain.

2. Summary

A special four grain arrangement in 3D makes it possible to determine the mobility m_{qp} of a grain boundary quadruple point. The corresponding theoretical concept is put forward. It is shown that the mobility of a quadruple point is reflected by a dimensionless criterion Λ_{qp} which relates the angle at the tip of a quadruple point to the quadruple point mobility m_{qp}, the mobility of the grain boundary triple junctions m_{tj} and the grain size a. If the mobility of a quadruple point (strictly speaking, the product $m_{qp}a$) does not affect the motion of the four adjoining boundaries, then $\Lambda_{qp} \to \infty$ and the equilibrium angle at the tip of the quadruple point $\theta_1 \to \pi/3$. In case that m_{qp} is small, the quadruple point drags grain boundary motion and in the limit $m_{qp} \to \infty$, $\Lambda_{qp} \to \infty$ and $\theta_1 \to 0$.

It is emphasized that an immobile quadruple point will pin a boundary system, i.e. suppress its motion since a migration of the whole boundary system by necessity requires that the boundaries, the triple junctions, and the quadruple point move jointly.

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