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A variational approach to the modelling of grooving in a three-dimensional setting

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ABSTRACT

We present a theory of thermal grooving, i.e. surface motion due to surface diffusion, based solely on geometrical and energetic arguments and a variational approach involving a thermodynamic extremal principle. The theory is derived for a fully three-dimensional setting. All interface and contact conditions at junction lines and points of the material aggregate are derived rigorously and without ambiguity. A finite element implementation of the model is employed. Numerical examples are presented and compared with experimental results from the literature.

1. Introduction and motivation

Kinetics of grooving, which occurs e.g. during thermal etching of polycrystals, has been studied by several authors since several decades. The shape of the grain surfaces is assumed to develop by surface diffusion driven by the gradient of surface curvature. A typical micrograph of a thermal groove is displayed in Fig. 1.

The majority of models used in simulations are developed for a two-dimensional setting and for a symmetric configuration with the grain boundary normal to the initially planar surface. Pioneering papers in this field were elaborated by Mullins [1,2]. Some decades later the Mullins concept was complemented by applying a travelling wave solution, see Refs. [3–5]. The dihedral angle in the groove root is given by the equilibrium of interface tensions (assumed to be equal to specific interface energies) in the grain boundary and in the surfaces. The dihedral angle and the continuity of the surface curvature define two contact conditions at the groove root. Furthermore, the surface flux at the groove root must be zero as no flux is assumed in the grain boundary. Boundary conditions at infinity are defined naturally. The situation gets more complicated, if the grain boundary is assumed not to be normal to the initially plane surface. Then one must distinguish between models accounting for a mobile or immobile grain boundary. The problem of interaction of free surfaces with a mobile grain boundary has been treated numerically by Svoboda and Riedel [6] for dragged pores and later by Zhang and Wong [7] for grooving. In both papers it is assumed that the tangent to the grain boundary at the triple junction halves the dihedral angle and that the curvature and surface flux are continuous there. The problem with an immobile grain boundary opens the question of values of contact angles at triple junctions. If the grain boundary halves the dihedral angle, there is one redundant contact condition at the triple junction. Further models for a two-dimensional setting shall be mentioned for surface and interface diffusion [7,8], grooves at singular surfaces and grain boundary sliding [9,10], grooves in thin filaments [11] and films [12]. Of particular interest have been two-dimensional models for the interaction of grooves with liquids [13,14].

The current solution concept is based on the Thermodynamic Extremal Principle, see Refs. [15–17] particularly for diffusive processes, for a three-dimensional setting. This variational study incorporates the whole system geometry and all participating energy terms and results in kinetic equations and proper contact conditions including one condition for contact angles. This solution procedure has already proven to be successful with respect to a

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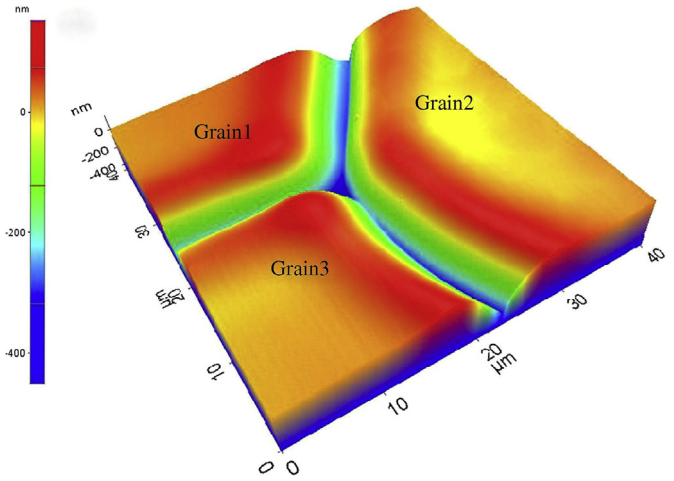

Fig. 1. Micrograph of thermal groove. Reproduced from Acta Mater., 58, Zhao, B., Verhasselt, J.Ch., Shvindlerman, L.S., Gottstein, G., Measurement of Grain Boundary Triple Line Energy in Copper, 5646–5653, 2010, Fig. 4, with permission from Elsevier.

two-dimensional setting or grooving [18,19] and grain growth and coarsening [20], allowing also for a limited triple junction mobility, see the contributions by Streitenberger and Zöllner [21,22]. However, one must keep in mind that modelling and simulation of grooving in a three-dimensional setting seem to be a new challenge. Only few papers dealt with this topic up to now. Here a series of papers by Gottstein and coauthors [23–28] has to be mentioned. The relevance of these contributions is based on the understanding of the triple line effects and measuring the triple line energy by using thermodynamically established relations for line energies. Furthermore, some simplified models describe the groove by a radially symmetric shape [5] or by a tetrahedron-like shape, see the recent papers [29,30]. It should be mentioned that also atomistic methods can be applied to model zones near triple junctions and consequently also near a quadruple junction, see the very recent paper [31] engaging the embedded-atom method. From the point of view of a rigorous three-dimensional treatment the work by Barret et al. [32], which appeared in the mathematical literature, should be mentioned. These authors already engaged a variational concept minimizing the Gibbs energy resulting in a three-dimensional finite element formulation of the groove. However, they assumed kinetic laws and contact conditions as given relations. We consider this as motivation to present a complete thermodynamically based three-dimensional model of grooving accounting for the following energy terms.

(i) the specific surface energy,
(ii) the specific grain boundary energy,
(iii) the line energy of the groove root,
(iv) the line energy of triple junction of three grain boundaries,

and for the following processes.

(i) surface diffusion,
(ii) diffusion along the groove root.

Kinetic laws and contact conditions are derived by the TEP from a general formulation of the problem. In addition, a concept for the numerical treatment of the kinetic laws respecting the contact conditions is provided.

2. Problem description

As system we consider the upper half of a thin polycrystalline layer with planar grain boundaries normal to the layer denoted as η_i. The grain boundaries meet in three grain boundary triple junctions denoted as Σ_i (-lines). The surfaces of individual grains are denoted as ω_i. The geometrical boundaries of these surfaces are denoted by $\partial\omega_i$. They meet each other and with grain boundaries in triple junctions denoted as Γ_i (-lines). The end-points of these lines are denoted by $\partial\Gamma_i$. The Γ_i- and Σ_i-lines meet in quadruple junctions P_i. A section of the system displaying a junction of three grains is depicted in Fig. 2.

2.1. Geometry and kinematics

We consider open surfaces ω_i with the normal vectors $\mathbf{n}_i$, which intersect along triple lines Γ_i with tangent vectors $\mathbf{t}_{\Gamma i}$, i.e. $\Gamma_i = \omega_j \cap \omega_k$ for appropriate j,k, see Fig. 2. Here we assume for simplicity that Γ_i lies in a plane, which may be the grain boundary, denoted as η_i, between two grains with the surfaces ω_j, ω_k. Within this plane Γ_i possesses an outward normal vector $\mathbf{n}_{\Gamma i}$. Moreover $\mathbf{m}_{\Gamma ij}$ is the unit vector at Γ_i in tangential direction of ω_j given by $\mathbf{m}_{\Gamma ij} = \pm \mathbf{t}_{\Gamma i} \times \mathbf{n}_j$, where the sign is chosen in such a way that $\mathbf{m}_{\Gamma ij}$ points away from Γ_i. Three (surface) triple lines and one (straight) internal triple line Σ_i meet at a quadruple point P_i, i.e. $P_i = \Sigma_i \cap \Gamma_j \cap \Gamma_k \cap \Gamma_l$ for appropriate j,k,l. The triple line Σ_i possesses an outward tangent vector $\mathbf{t}_{\Sigma i}$. For later reference, let us denote the set of all surfaces by $\mathbb{S}$, the set of all triple lines by $\mathbb{T}$, and the set of all quadruple points by $\mathbb{Q}$. We denote the set of all surfaces $\omega_j \in \mathbb{S}$ adjacent to a triple line Γ_i by

$$\mathbb{A}_{\Gamma i} = \{\omega_j \in \mathbb{S} | \Gamma_i \subset \partial\omega_j\}. \tag{1}$$

In the same manner let us denote the set of all triple lines $\Gamma_j \in \mathbb{T}$ adjacent to a quadruple point P_i by

$$\mathbb{A}_{Pi} = \{\Gamma_j \in \mathbb{T} | P_i \subset \partial\Gamma_j\}. \tag{2}$$

The velocity vector of a material point in the surface ω_i has a normal component $v_{n,i}$ measured as positive in direction of $\mathbf{n}_i$.

Let us assume now that Γ_i moves within the plane η_i with velocity $v_{\Gamma n,i}$, measured as positive in direction of $\mathbf{n}_{\Gamma i}$, see Fig. 3. The compatibility of an adjacent surface $\omega_j \in \mathbb{A}_{\Gamma i}$ at Γ_i enforces

$$v_{\Gamma n,i} = \frac{v_{n,j}}{\sin \alpha_{ij}}, \tag{3}$$

where α_{ij} denotes the angle between $\mathbf{n}_{\Gamma i}$ and $\mathbf{n}_j$, see Fig. 3. A positive motion of Γ_i leads to a reduction of the area A_j of the adjacent surface ω_j via the tangential velocity $v_{t,j}$. From Fig. 3 we deduct

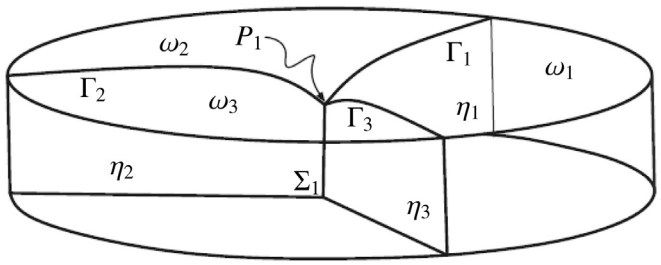

Fig. 2. A part of the system showing the groove geometry and geometrical elements for three adjacent grains.