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Influence of accounting for translational motion of grains on grain growth kinetics and size distribution

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ABSTRACT

The thermodynamic dissipation-based approach, being one of the approved effective methods for treatment of grain growth, is refined by accounting for dissipation due to translational motion of individual grains during grain growth. The present model introduces an interaction function correlating the velocity of translational motion and the rate of growth for individual grains. The comparison of results of simulations based on the present model with existing phase-field simulations indicates that about 1/4 to 1/3 of the driving force is dissipated by translational motion of grains lowering the grain growth kinetics and changing of the steady state grain radii distribution function.

Grain growth, in its original description, is studied by change of the effective radii R_i of grains in an ensemble of N grains due to the reduction of the total grain boundary energy. The rate $\dot{R}_i$ follows, as in the seminal works by Hillert [1,2], the classical evolution law

$$\dot{R}_i = \alpha_H \gamma M (1/R_C - 1/R_i), \tag{1}$$

with γ as specific value of the grain boundary energy, M as mobility of the grain boundary and a kinetic factor $\alpha_H \approx 1$, the value of which has been estimated heuristically. The quantity R_C is denoted as critical radius yielding the grains with $R_i < R_C$ to shrink and with $R_i > R_C$ to grow. The critical radius R_C can be calculated by using the condition of constant total volume of grains enforcing for spherical grains and inserting of Eq. (1) as

$$\sum_{i=1}^{N} R_i^2 \dot{R}_i = 0 \quad \Rightarrow \quad R_C = \sum_{i=1}^{N} R_i^2 / \sum_{i=1}^{N} R_i. \tag{2}$$

Approx. 40 years later the authors of this paper derived the same equation as Hillert in [3] by application of Thermodynamic Extremal Principle (TEP) (for details see, e.g., [4,5] for its original formulation and [6] for its advanced and more detailed formulation). However, the kinetic factor has followed as $\alpha_{TEP} = 2 \approx 2\alpha_H$. Recently Kertsch and Helm [7] investigated the grain growth problem by employing Rational Extended Thermodynamics and obtained an evolution equation equivalent to Eq. (1) with $\alpha_{K-H} = 2$. Common to both approaches ([3,7]) is the fact that only radial motion of grains is considered, i.e. either as their expansion or shrinking. However, the authors of this paper argued already in [3] that α_{TEP} is obviously too high (by factor of about 2), since the translational motion of centers of the individual grains, being also a dissipative process inevitably accompanying grain growth, is not taken into account in the thermodynamic concepts.

One must admit that the models, based on approximation of grains by spheres of effective radii and on the mean field approach, cannot treat the grain growth perfectly. Each 3-D grain has a rather complex shape as a polyhedron with uneven faces. The non-zero curvatures of the faces drive grain boundary migration and provoke grain growth.

A polycrystal can be considered as a set of zones (i.e. grains) in an arrangement of macroscopically fixed atoms separated by mobile boundaries (the motion of atoms due to rearrangement of atoms in the migrating grain boundary is negligible). Thus, during the grain boundary migration the mass does not move and the individual grains evolve as they contain different atoms, or, in other words, they are defined by changing zones. So, beside the volume changes of grains the grain boundary migration leads also to changes of the shapes of the grains as well as to the changes of their positions. The last one, i.e. translational motion of the grain, is driven by a generally unbalanced (non-zero) total tension of grain boundaries adjacent to the grain. A grain evolving in a polycrystal may change only its shape and position without changing its volume. As a simple example one

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can mention that all grains with 6 neighbours in the 2-D grain structures behave in such a way, see the seminal paper by Mullins [8]. To the best knowledge of the authors, this translational motion of the grains has not been considered in the open literature yet. This motion differs to the grain translation in crystals due to climbing grain boundary dislocations and/or deposition or removing of atoms at grain boundary causing relative motion of lattices of adjacent grains as treated e.g. in [9].

It is hardly imaginable, how the translational motion of grains embedded in a polycrystal can be experimentally detected and evaluated. Within this context phase field studies can be considered as "computer experiments". As pioneering work the study by McKenna et al. [10] can be considered offering a comparison between phase field simulation and experiments. The translational motion of grains is, however, not evaluated in this study. With respect to the kinetic factor α and grain size distribution function the studies by Kamachali et al. [11,12] shall be mentioned. Obviously it was simply assumed in the thermodynamic models, see the discussion concerning α_H above, that nearly one half of the grain boundary energy dissipates by translational motion of grains and/or their shape change, which only slows down the kinetics of growth as given by Eq. (1). This assumption, however, deserves a detailed analysis. Thus, the question is still open, how the both motions (radial and translational) interact and how the interaction can be effectively accounted for in thermodynamic models for grain growth.

It should be mentioned that also other phenomena accompanying grain growth have already been included in the models of grain growth. Cahn and Taylor published a detailed study [13] on the relative sliding of grains along grain boundaries provoked by grain rotation. These authors formulated constitutive equations for the normal and tangential growth velocity, which were confirmed to a certain amount also by experiments, see, e.g., [14]. The mentioned constitutive equations in [13] were recently extended in [15] and particularly applied with respect to the kinetics of junctions in [13]. Furthermore, the configuration, as introduced in [13], was involved in a Phase-Field Crystal study [9] and very recently improved in [16] by taking into account motion of triple junctions. Also a German group [17] recovered predictions of Cahn and Taylor by modelling of grain boundary dynamics within an amplitude equations description. One must, however, keep in mind that in the unloaded systems the driving force for grain boundary sliding and rotation of grains stems from the dependence of specific grain boundary energy γ on grain orientation by keeping the total grain boundary area fixed. This contradicts our assumptions taking the value of specific grain boundary energy γ as a fixed quantity and the driving force stemming from the decrease of the total area of grain boundaries.

In the actual grain growth models based on the energy balance in the system, see [3,7], the 3-D grains are approximated by spheres of effective radii within the mean field approach (not taking care of the positions of the grains in the system). Then the change of the shapes and positions of the grains are not accounted, although they dissipate a part the grain boundary energy. As these dissipation processes are not included in the actual grain growth models, they overestimate the kinetics. The goal of our paper is now to extend the established thermodynamic concepts for grain growth [3,7] by accounting the translational motion of individual grains and show its influence on grain growth kinetics and steady-state grain size distribution function.

As first step we deal with the energetics of grain growth with grain translation. The total Gibbs energy G of the system, see also [3], Sect. 2, can be expressed by approximating grains in the polycrystal by spheres of effective radii R_i as

$$G = 2\pi\gamma \sum_{i=1}^{N} R_i^2. \tag{3}$$

The rate $\dot{G}$ of G delivers directly the dissipation D of the system, see [4] and particularly, for discrete quantities as R_i see [4,18], since the grain radii R_i can be considered as internal variables with their rates $\dot{R}_i$, as.

$$D = -\sum_{i=1}^{N} \frac{\partial G}{\partial R_i}\dot{R}_i \text{ with } \frac{\partial G}{\partial R_i} = 4\pi\gamma R_i. \tag{4}$$

We assume that each grain evolves by its expansion/shrinking rate $\dot{R}_i$ and also by translational movability of its centre by velocity V_i. Thus, the dissipation function Q consists of two contributions: Q_R due to the expansion or shrinking of individual grains and Q_T due to their translational motion. The contribution Q_R can directly be taken from [3], Sect. 2 as

$$Q_R = \frac{2\pi}{M}\sum_{i=1}^{N} R_i^2 \dot{R}_i^2. \tag{5}$$

The contribution Q_T is assigned to the dissipation due to the grain boundary migration by a normal velocity v_i, being the projection of the translational velocity V_i on the surface normal. With the value $v_i = V_i \sin\theta\cos\psi$, using spherical coordinates, the dissipation related to a grain boundary element $\mathrm{d}A = R^2 \sin\theta \mathrm{d}\varphi \mathrm{d}\theta$, is proportional to $v_i^2 \mathrm{d}A$. Integration over the grain boundary results after some analysis as

$$Q_T = \frac{4\pi}{3M}\sum_{i=1}^{N} R_i^2 V_i^2. \tag{6}$$

Then the total dissipation function follows as

$$Q = Q_R + Q_T = \frac{2\pi}{M}\sum_{i=1}^{N} R_i^2\left(\dot{R}_i^2 + aV_i^2\right), \tag{7}$$

with $a = 2/3$ being a geometry factor.

Since the dissipation D (see Eq. (4)) does not involve V_i, the driving force for V_i must stem from geometry of the system expressing the fact that translation of grains is an inherent phenomenon accompanying grain growth in polycrystals. Thus one must make an assumption how V_i and $\dot{R}_i$ are correlated. Obviously V_i of the largest grains can be assumed to be rather small as their expansion on the account of surrounding smaller grains is nearly isotropic. Contrarily, for grains, which practically do not expand/shrink (with the radius $R_i \approx R_C$), V_i should assume a nearly constant value. Consequently, we suggest a relation (interaction function), which meets such behaviour,

$$V_i^2 = b\frac{R_C^2}{(R_i - R_C)^2}\dot{R}_i^2, \tag{8}$$

with b being a grain-structure inherent property and the product ab is taken as system parameter. If one inserts Eq. (1) in Eq. (8), one can realize that for $R_i \to R_C$ the quantity V_i really assumes a nearly constant value and for large grains V_i decreases as it scales with $1/R_i^2$. Moreover, for $R_i \to 0$ the quantity V_i scales with $1/R_i$ or $\dot{R}_i$, which is also acceptable, as the translational movability of grains increases with decreasing radius. Then the dissipation function Q, Eq. (6), can be written by inserting of Eq. (8) into Eq. (7) as

$$Q = Q_R + Q_T = \frac{2\pi}{M}\sum_{i=1}^{N} R_i^2\dot{R}_i^2\left(1 + ab\frac{R_C^2}{(R_i - R_C)^2}\right). \tag{9}$$

Finally, we introduce a weighting factor κ between Q_R and Q_T as $Q_R = \kappa Q_T$. This factor κ expresses the relation between dissipation by grain growth and translational motion of grains and so explains the discrepancy e.g. between α_H and α_{TEP}. The factor κ is taken as parameter of