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The envelope of size distributions in Ostwald ripening and grain growth

Peter Streitenberger* and Dana Zöllner

Institute for Experimental Physics, Otto von Guericke University Magdeburg, PO Box 4120, 39016 Magdeburg, Germany

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Abstract—In the present paper the scaling properties of microstructure coarsening by Ostwald ripening or grain growth are studied by means of the envelope of the family of evolving size distribution functions, which complements the usual scaling analysis by some new aspects and results. For a self-similar family of size distribution functions the envelope is uniquely determined by the growth exponent and an envelope parameter, where the latter is a new characteristic quantity of the coarsening system associated with the scaled size distribution function. If the family of size distributions obeys the continuity equation their envelope is the location of the maximum particle flux density in size space, while for the corresponding cumulative size distribution the envelope is the location of maximum size that a particle or grain can take during the passage through its growth path. The construction of the envelope curve therefore allows the independent determination of some coarsening parameters without recourse to the full time development of the individual growth paths. Numerical studies by means of the Monte Carlo Potts model of grain growth confirm and complement the analytical results. Especially they reveal that at the early stage of growth the envelope has a much reduced and non-integer exponent.

Keywords: Coarsening; Ostwald ripening; Grain growth; Size distribution function; Envelope

1. Introduction

Size distributions of particles and grains in materials are important quantities for the characterization of materials microstructures and their time development during coarsening. It is basically understood that not only the average particle or grain size but also its stochastic counterpart, the size distribution function, influences many microstructure–property relationships of materials (compare, e.g., [1–3]). What is no less important, the time variation of the size distribution function itself also provides information on the basic physical processes underlying the coarsening kinetics of the microstructure considered. This is especially evident in the scaling properties of the size distribution function, the subject of many studies in recent years especially for Ostwald ripening (e.g., [4–7] and the literature within) and grain growth (e.g., [8–11] and the literature within). The present paper deals also with this problem, but in contrast to the above works we consider a property of the size distribution function that has not been studied so well in this context, namely the envelope of a set of temporally developing size distribution functions.

Before we deal with it in more detail, let us first briefly review the scaling properties of the size distribution function of the coarsening systems under consideration. To that aim we define the size distribution function (from now on referred to SDF), $F(R,t)$, as usual in such a way that $dN = F(R,t)dR$ is the number of particles or grains per unit volume at time t and size interval dR (cf., e.g., [1,6]). For an evolving microstructure the SDF represents in a $F(R,t)$ vs. R plot a family of curves with time t as the family parameter (Fig. 1a) [12]. In the important case of scale coarsening as it is the case for Ostwald ripening and normal grain growth the set of SDFs shown in Fig. 1a can be represented by the function

$$F(R,t) = g(t)\cdot f(x) = \frac{A}{l^{\alpha}} f\left(\frac{R}{l}\right), \tag{1}$$

which separates in a purely time dependent function $g(t) = \frac{A}{l^{\alpha}}$ and a scaled SDF $f(x) = f\left(\frac{R}{l}\right)$ that depends only on the relative size variable $x = \frac{R}{l}$ [4–7]. As the typical scaling length l of the system often the directly measurable average particle or grain size is used. The scaling exponent α can take both non-integer and integer values; the latter is the case for the quasi-stationary state in volume- or mass-preserving coarsening (see below). Non-integer α-values can be found for example in coarsening of fractal systems [13]. The scaling length $l = l(t)$ follows a power-law of the form

$$l = \left(kt + l_0^{1/\beta}\right)^{\beta}. \tag{2}$$

The growth exponent β characterizes the underlying dynamics typically for the observed coarsening kinetics, where $\beta = 1/3$ for diffusion controlled Ostwald ripening

* Corresponding author. Tel.: +49 (0) 3916758581; fax: +49 (0) 3916718108; e-mail addresses: peter.streitenberger@ovgu.de; dana.zoellner@ovgu.de

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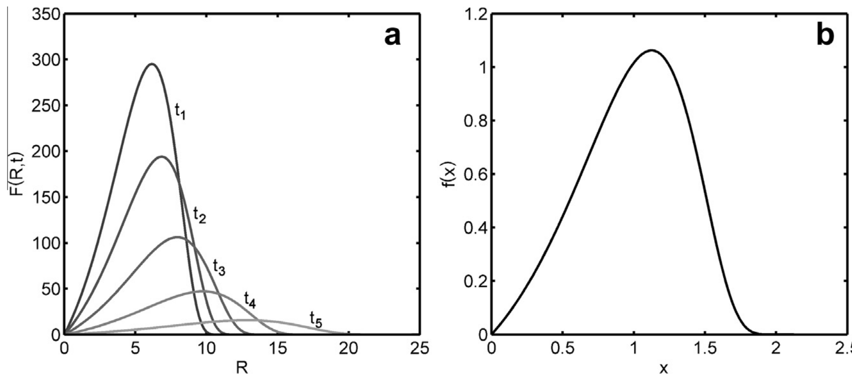

Fig. 1. (a) Family of size distribution functions $F(R,t)$ of an evolving microstructure with time t as the family parameter with $t_1 < t_2 < t_3 < t_4 < t_5$. (b) Scaled SDF $f(x) = f(R/l)$ according to Eq. (1).

and $\beta = 1/2$ for interface controlled Ostwald ripening and curvature driven grain growth [4,5,14]. Under this scaling hypothesis the family of SDFs in Fig. 1a collapses to a unique single curve as shown in Fig. 1b. Therefore, the whole family of SDFs in Fig. 1 can be described by a single, time-independent scaled SDF $f(x)$ that is characteristic for the type of coarsening process and possibly also of other properties of the microstructure and the time law Eq. (2) of the associated scaling length.

The theoretical basis of the scaling theory of Ostwald ripening and polycrystalline grain growth was laid by Lifshitz, Sloyzov and Wagner (LSW) [15,16] and Hillert [17], respectively. In particular, in these seminal works the connection between the SDF and the governing growth law via the continuity equation in size space has been established and analyzed under the scaling assumption, Eq. (1). These and subsequent developments of this approach to coarsening theory can be found in recent reviews and papers such as for the Ostwald ripening theory including the important extensions to non-zero volume fraction of the second phase, e.g., in [5–7,18,19] and for grain growth theory including the consideration of the grain size-topology correlation, e.g., in [8–11,20–22].

Of the developments that should be highlighted here are those that are specifically concerned with the general relationships between the different types of SDFs and the growth law and which are particular relevant to the present paper. The scaling hypothesis has been generalized to the statistical self-similarity hypothesis by Mullins [4,14] summarizing many investigations of grain growth and coarsening under a single scheme. Assuming this scaling hypothesis, the relationship between the SDF and the growth law calculating the SDF from the growth law and vice-versa was treated by Hunderi and Ryum [23], Grätz [24,25], Mullins [9], Vinals and Mullins [26] and Stevens and Davies [27]. The inverse relationship giving the growth law of coarsening from the SDF was also studied recently by means of a thermodynamic variational principle by Svoboda and Fischer [28] and Fischer et al. [29]. Regarding the cumulative SDF DeHoff [30] and, independently, Woodhead [31] have developed a graphical method that allows obtaining the growth law from time sequences of cumulative SDF. This method was applied to particle coarsening by Fang et al. [32] and studied theoretically by Yost [33] and Grätz [25] on the basis of the LSW theory.

In the present paper, a further time-independent scaling relationship of the SDF is considered, which has not yet been studied in detail, namely the envelope curve of a family of SDFs such as shown in Fig. 1a. To the best of our knowledge, the only application of the envelope curve of a set of SDFs of an evolving coarsening system exists in the recent papers by Loureiro et al. [34,35]. Therein the envelope of an area size distribution function has been used as a way to obtain numerically the characteristic length scale in the considered system of a q-states Potts model. In contrast, we consider in the present work for the first time the analytical properties of the envelope of evolving SDFs of the classical coarsening theory. In particular, a new parameter is introduced, which determines uniquely the envelope of the family of SDFs, Eq. (1), defined by the scaled SDF $f(x)$. The analysis of the envelope of the evolving SDF provides some interesting new aspects of coarsening kinetics and thus complements the above works for coarsening theory. We would like to point out that the envelope considered here should not be confused with the so-called growth path envelope analysis of DeHoff [30]. The relationship with the latter is considered in chapter 4 in connection with the cumulative SDF.

The paper is organized as follows. In the next chapter the general equation of the envelope of a self-similar set of SDFs is derived and used to characterize their scaling properties. By deriving the envelope parameter for the LSW distribution functions and others some new results are presented for the classical coarsening theory. In chapter 3, the relationship between the envelope of the SDF and the associated continuity equation is examined, while in chapter 4 the envelope of the cumulative SDF is considered. At this point also a connection to the growth path envelope analysis of DeHoff is made. Finally, in chapter 5, numerical studies for the determination of the envelope using the Monte Carlo Potts model for grain growth are presented confirming the theoretical results and revealing interesting new scaling properties of the envelope in the early stage of coarsening.

2. The envelope of a family of size distributions

Considering the family of SDFs $F(R,t)$ as shown in Fig. 1 with time t as the family parameter, the envelope $F_e = F_e(R)$, that is the curve which touches all members of the given family of curves, is defined by the following set of equations [36]:

$$\Psi(F_e, R, t) = 0, \tag{3a}$$