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ScienceDirect

Acta Materialia 90 (2015) 10–26

Acta MATERIALIA

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Effect of initial particle size distribution on the dynamics of transient Ostwald ripening: A phase field study

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Received 26 January 2015; revised 14 February 2015; accepted 16 February 2015
Available online 3 March 2015

Abstract—The coarsening of polydisperse particles with different initial particle size distributions (PSD) is studied using a quantitative phase field model in two dimensions with emphasis on the transient behavior before reaching steady state. The coarsening rate constant, scaled PSD, scaled evolution law and radial distribution function were systematically examined and compared with available theoretical and experimental results. It is found that the length of transient regime is directly correlated with the extension of the initial scaled PSD toward the large particle size region, i.e. the so called tail, rather than the width of scaled PSD which can be described in terms of standard deviation. Initial distributions with short tails evolve rapidly to the steady state even though the initial width of PSD is large. Whereas, after long time coarsening with a factor of 4–6 change in average radius, initial distributions with long tails still deviate from the steady-state form, yet may appear stable due to the slowly changing rate. Some inconsistencies about the transient coarsening behaviors in previous studies are clarified based on the present results. Moreover, the validity of circular shape assumption is certified when the particle volume fraction is not larger than 0.4.
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Keywords: Ostwald ripening; Phase field model; Phase transformation

1. Introduction

Ostwald ripening, or particle coarsening, is a common kinetic phenomenon which occurs in the polydisperse two-phase mixture via a diffusive mass flow from small particles to large ones. This process results in a substantial increase in the average particle size and a corresponding decrease in the particle number density. A better understanding of this process is of great fundamental and practical interest.

Since the first quantitative analysis by Lifshitz and Slyozov [1] and by Wagner [2] (LSW), numerous modified theories [3–22] have been developed to describe the kinetics of Ostwald ripening process. A collective objective of all these theories is to find a proper kinetic equation describing the averaged growth rate of a particle with a given size. Once this is determined, the dynamics of coarsening process can be completely defined by combining with the continuity equation for particle size distribution and the mass conservation law. The kinetic equation in LSW theory is only valid in the case of vanishing volume fraction (f_v). Taking into account the effect of interparticle diffusional interaction at nonzero volume fraction has been the major objective of modern coarsening theory. The existing approaches to address this issue can be classified into two categories: (i) mean-field description based on some ad hoc assumptions [3–8] or taking into account diffusion screening [9–12]; (ii) microscopic description that represents the mass flow from each particle as a monopole source or sink, employing statistical mechanical methods [13–16] or computer simulation [17–22] to determine the averaged quantity of interest. All these theories carried out analysis strictly only in the long time limit, where the system approaches to a scaling regime (steady state). In this regime, the particle size distribution (PSD) is time independent, or self-similar, when scaled by the average radius. The average radius, $<R>$, grows with time, t, according to:

$$\langle R(t)\rangle^3 - \langle R(t_0)\rangle^3 = Kt \tag{1}$$

where $<R(t_0)>$ is the average radius at initial time t_0 and K is the coarsening rate constant depending on the volume fraction of particles and material parameters.

All of the aforementioned theories except those employing numerical simulations are strictly valid only in the long time limit. Their applicability to practical coarsening process with finite time is hinged on the assumption that the evolution to steady state in experiments is rapid rather than taking infinite long time. This assumption has been widely accepted since the scaled PSD seemed to be self-similar within finite experimental time. However, this viewpoint has been discredited by a series of careful experiments carried out by Voorhees and coworkers in microgravity environments of space shuttle [23–25], which is the most

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http://dx.doi.org/10.1016/j.actamat.2015.02.030
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accurate experimental test of theory by far. They found that even though the average radius changed by a factor of three, the measured data still deviated from predictions of all theories for steady-state regime, but agreed well with simulations taking into account the transient coarsening. Through carefully reexamining former experiments in light of transient coarsening [25], they concluded that the seemly time independent scaled PSD observed in many experiments does not mean an actual presence of steady state, and the transient stage may be so long that the steady-state theories are inadequate to describe the practical coarsening behavior. These results indicate a great importance to ascertain the dynamics of coarsening in the transient regime.

Theoretical work on transient coarsening is rather limited compared with the great efforts to account for the effect of finite volume fraction. Getting an analytical solution of the fully time dependent coarsening problem is a formidable task. The existing studies in the transient regime employed either the numerical calculation of mean-field model [26–29] or the simulation based on the microscopic description of coarsening process [17,25,30]. Through these studies, it has been confirmed that: (i) the evolution path of scaled PSD toward the asymptotic state is not constrained, but remarkably affected by initial conditions; (ii) the LSW PSD is a unique attractor state in the limit of zero volume fraction; and (iii) wide distributions coarsen more rapidly than narrow ones. However, the present understanding of transient coarsening behavior is still not satisfactory, especially in the effect of the initial shape of scaled PSD on the length of transient stage. The numerical calculations by Enomoto et al. [27] showed that the initial width of scaled PSD had no observable effect on the length of transient stage, while other studies [17,29,30] exhibit clear correlations between the initial width of distribution and the duration of transient stage. Voorhees and Glicksman [17] and Smet et al. [30] found that the transient stage for initial wide distributions was longer than that for the narrow ones. Whereas Chen and Voorhees [29] found that at the end of their calculation the PSD which is initially the widest of three different distributions is the closest to the steady-state form, which means the transient stage for the initial widest distributions may be the shortest. Besides the effect of the initial width of scaled PSD, the initial tail of scaled PSD, i.e. the extension of PSD toward the large particle size region, is also found to have an effect on the rate of approach toward steady state [28,29]. Usually the tail of PSD is correlated with the width of PSD, i.e., wide PSDs possess long tails. But the tail of PSD can also change independently. It is not clear which of the two effects is more significant in determining the length of transient stage. Moreover, different evolution paths of initial narrow PSDs toward steady-state form have been observed. It was found by Chen and Voorhees [29] and Venzl [26] that in the limit of zero volume fraction, the initial narrow PSDs became wider than the steady-state PSD at first and then narrowed toward the final form. However, the studies of Enomoto et al. [27] and Fang et al. [28] showed that at a finite volume fraction, the initial narrow PSDs widened monotonically toward the asymptotic distributions. Thus it is still not clear whether non-monotonic evolution of the initial narrow PSD will happen at finite volume fractions. Besides, the effect of volume fractions on the length of transient stage is also inconsistent in different studies. Chen and Voorhees [29] found systems with finite volume fractions of coarsening phase evolved to the steady state more rapidly than do systems with zero volume fractions, whereas by comparing experimental results with transient simulations Snyder et al. [25] concluded that the time required to reach steady state increases with increasing volume fractions. It should be noted that these former studies on transient coarsening have used very different simulation approaches and various types of initial PSDs. Both of these two factors may account for the above mentioned inconsistencies. More accurate simulation approach and more systematical studies with various initial PSDs are still needed to further explore the transient coarsening behavior and clarify the existing inconsistencies.

All the previous theoretical studies of coarsening [1–30] are based on the assumption of spherical or circular particle shape, which is only valid at a small volume fraction. In order to avoid such an artificial geometrical assumption, the phase field model is a suitable choice, since the long range diffusion and particle shape accommodation due to solute interaction can be automatically taken into account in this model. Phase field simulations of particle coarsening have been carried out firstly by Warren and Murray [31] and Conti et al. [32]. Due to the restricted time and size scales, they cannot make any quantitative comparison with available theories, but have demonstrated the potential of phase field model in the study of coarsening. Then Diepers et al. [33] and Ode et al. [34] further extended the phase field simulation to a large scale and found an agreement with previous theoretical studies in the range of small volume fractions ($f_p < 0.2$). Since the difference of particle orientation is not considered in these earlier simulations, particle coalescence is inevitable especially when the particle volume fraction is high. Recently, phase field simulations taking into account particle orientation have been preformed by Fan et al. [35] and Kim [36] at high volume fractions ($0.2 < f_p < 0.9$) and by Wang et al. [37,38] at ultrahigh volume fractions ($f_p > 0.9$), and have been extended to multi-component systems by Mukherjee et al. [39]. There are also many simulations for coarsening in coherent solids [40–46], where elastic energy plays an important role. The primary intention of all the existing phase field simulations of coarsening is to investigate the kinetics in steady state and illustrate the effect of volume fractions and/or elastic stress. An approximately time-independent scaled PSD has been considered as an indication of achieving steady state. However it may be also due to the slow rate of change toward steady state. Whether a truly steady state has been reached was never carefully examined in these studies, and there is no emphasis on the transient coarsening behaviors using the phase field method as far as we know.

In this paper, we present a systematic study of the effect of the initial scaled PSD on the transient coarsening behaviors by the phase field simulations over a wide range of volume fractions. A series of initial scaled PSDs were investigated in order to distinguish the effects of the initial width of PSD and of the initial tail of PSD. The results of simulations were compared with theoretical and experimental results. Some inconsistent viewpoints about transient coarsening behavior are clarified based on present studies. Moreover, the circular shape assumption used in theoretical models of coarsening is assessed for system with high volume fractions.

The structure of this paper is as follows. Section 2 introduces the phase field model, the distribution function used to generate the initial PSD and the simulation parameters.

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