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An extension of mean-field coarsening theory to include particle coalescence using nearest-neighbour functions

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ABSTRACT

A mean field description of particle coalescence and Ostwald ripening is presented. The inclusion of particle coalescence events is shown to influence the evolution of the size distribution function and the time taken to reach the steady state particle coarsening regime. Nearest neighbour functions are used to represent the spatial arrangement of particles within multi-modal particle radius distributions and to calculate the frequency of coalescence events. The impact of particle coalescence upon long term coarsening kinetics has been studied. By tracking the evolution of a unimodal and bimodal dispersions in phase space, it is demonstrated that coalescence affects the paths of particle dispersion towards the steady state particle coarsening regime as well as the time scales to reach it.

1. Introduction

The mechanical response of precipitate strengthened alloys are significantly influenced by the size and spatial distribution of the embedded particle phase. At high temperatures the dispersion is unstable, with particle growth rates driven by the minimisation of the free energy. During Oswald ripening, kinetics of particle coarsening are driven by the minimisation of the interfacial energy between the particle and matrix phases. This phenomena was first treated by Greenwood [1] and later expanded into a comprehensive mean field theory by Lifshitz and Slyozov [2] and Wagner [3] (LSW) for dilute particle dispersions in a binary alloy. LSW coarsening theory predicts the existence of an attractor (steady) state for the particle radius distribution. Once such a state is attained LSW theory predicts scaling laws for the temporal evolution of the moments of the particle size distribution: the cubed mean particle radius increases linearly with time and the concentration of particles decreases linearly with time.

Over the last forty to fifty years, there has been a considerable effort on the extension of LSW coarsening theory to describe particle kinetics in engineering precipitate strengthened materials. Progress has been made in linking the chemical composition of alloys to coarsening kinetics through CALPHAD (Computer Coupling of Phase Diagrams and Thermochemistry) [4]. Kheuman and Voorhees [5] developed a description of ternary alloys, which was later generalised to multi-components by Jou et al. [6] and Phillipe and Voorhees [7]. Other multi-component formulations have been developed such as that by Svoboda et al. [8] and Chen et al. [9]. Software such as TC PRISMA [10] and MatCalc [11] offer the ability to calculate the phase diagram, particle composition, thermodynamic variables and mobility variables needed to determine the particle kinetics as a function of chemical composition. These models capture the formation and growth of particles, describing Ostwald ripening kinetics coupled with classical nucleation theory.

Another key aspect in simulating the precipitate kinetics in engineering alloys is the treatment of non-dilute particle systems [12]. Neighbouring particle's diffusion fields may interact, accelerating the particle growth or dissolution rate. Multiple-particle diffusion has been assessed by describing the diffusion field as quasi-static with particles treated as either point sources or sinks [13–15]. Several authors have built upon this approach and that of Ardell [12], deriving correction factors to modify dilute particle growth rates to describe finite volume fraction particle dispersions [16–18].

Other phenomena may impact particle coarsening behaviour such as changes in particle morphology [19,20], inverse coarsening [21] and particle coalescence [22]. Differences in lattice parameter between coherent particles and matrix gives rise to

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misfit stresses which contribute to the elastic strain energy and influences the particle morphology [19]. When the contribution to the total energy of elastic strain energy is greater than that of interfacial energy, it is possible that small particles grow at the expense of larger particles. Su et al. [21] describe such events as inverse coarsening. In high volume fraction particle dispersions, particle coalescence can impact both particle morphology and size [22].

The aim of this paper is to further develop the mean field description of population dynamics of polydispersed particles to include coalescence events. The approach involves introducing appropriate coalescence source and sink terms to the advection differential equation governing the evolution of the particle size distribution and is developed in Section 2. To account for the spatial arrangement of particles, a statistical approach based on nearest neighbour functions has been adopted. Numerical implementation of the model is outlined in Section 3. The results and discussion sections are given in Sections 4 and 5, and the work is concluded in Section 6.

2. A mean field description of particle coarsening and coalescence

2.1. Evolution of the particle radius distribution

The particle radius distribution function $F(R,t)$ is defined as follows: the number of particles per unit volume with radius between R and $R + dR$ is given by $F(R,t)dR$. The total number of particles per unit volume $N_v(t)$ is then the integral of this function for all possible particle radii

$$N_v(t) = \int_0^\infty F(R,t)\, dR \tag{1}$$

Nucleation, dissolution and coalescence of particles will influence the temporal evolution of $N_v(t)$. These mechanisms can be accounted for by introducing appropriate source and sink terms, such that the rate of change of the total number of particles per unit volume is given by

$$\dot{N}_v(t) = \dot{N}_v^+(t) - \dot{N}_v^-(t) \tag{2}$$

where $\dot{N}_v^+(t)$ and $\dot{N}_v^-(t)$ are the 'generation' and 'removal' rates, respectively. These are associated with a number of possible phenomena such as nucleation, coalescence and dissolution. Both $\dot{N}_v^+(t)$ and $\dot{N}_v^-(t)$ can be expressed in terms of particle size density functions $\dot{n}^+(R,t)$ and $\dot{n}^-(R,t)$, so that the number of particles generated and removed per unit volume with radius lying in the closed interval $[R,R + dR]$ is then $d\dot{N}^+ = \dot{n}^+(R,t)dR$ and $d\dot{N}^- = \dot{n}^-(R,t)dR$. With these definitions, Equation (2) becomes

$$\dot{N}_v(t) = \int_0^\infty \left(\dot{n}^+(R,t) - \dot{n}^-(R,t)\right) dR \tag{3}$$

The source terms $\dot{n}^+(R,t)$ and $\dot{n}^-(R,t)$ may be introduced into the continuity equation:

$$\frac{\partial F(R,t)}{\partial t} + \frac{\partial (F(R,t)V(R,t))}{\partial R} = \dot{n}^+(R,t) - \dot{n}^-(R,t) \tag{4}$$

From the moments of $F(R,t)$ the mean particle size and volume fraction of the dispersion can be calculated:

$$\left\langle R \right\rangle = \frac{1}{N_v}\int_0^\infty R\, F(R,t) dR \tag{5}$$

$$\phi = \frac{4}{3}\pi \int_0^\infty R^3 F(R,t) dR \tag{6}$$

The general form of the particle growth rate for spherical particles is given by Ref. [23].

$$V(R,t) = \frac{A(t)}{R}\left(\frac{1}{R_c(t)} - \frac{1}{R}\right) z(R,t) \tag{7}$$

where A is a function of the diffusivities of the alloying elements. The term z is a correction factor that accounts for competitive growth [12–18]. The parameter R_c is a critical radius and represents the particle size at which the transition between dissolution and growth occurs. The mean field description outlined above assumes that particles are spherical and maintain this morphology as the particle radius distribution evolves.

2.2. Particle coalescence

Consider the coalescence of two particles of size R_1 and R_2 forming a new particle of size R. Introducing the volume fraction frequency density $g(R,t)$ defined such that the volume fraction of particles having radius between R and $R + dR$ is $g(R,t)dR$. This is the probability of finding particles with radius lying in the closed interval $[R,R + dR]$. It is related to the distribution function $F(R,t)$ as follows

$$g(R,t)dR = \frac{4\pi}{3} F(R,t) R^3 dR \tag{8}$$

Assuming that the probability of any two particles randomly sampled from the dispersion having sizes R_1 and R_2 are independent from each other, then the likelihood of the first particle having a radius $R_1 \in [R_1, R_1 + dR_1]$ and the second particle having a radius in $R_2 \in [R_2, R_2 + dR_2]$ is given by $g(R_1,t)$,$g(R_2,t)dR_1dR_2$. Let $G_p(R_1,R_2,\lambda)$ be a spatial distribution function (to be defined in Section 2.3) such that the probability of finding a particle of size R_1 at a distance $[\lambda,\lambda + d\lambda]$ from R_2 is given by $G_p(R_1,R_2,\lambda)d\lambda$. The probability of two particles with radius $R_1 \in [R_1', R_1' + dR_1']$ and $R_2 \in [R_2', R_2' + dR_2']$ a distance $\lambda \in [\lambda', \lambda' + d\lambda']$ is

$$\begin{aligned} P\left[R_1' < R_1 \le R_1' + dR_1', R_2' < R_2 \le R_2' + dR_2', \lambda' < \lambda \le \lambda' + d\lambda'\right] \\ = f_c(R_1', R_2', \lambda') dR_1' dR_2' d\lambda' \end{aligned} \tag{9}$$

where

$$f_c(R_1', R_2', \lambda') = g(R_1', t) g(R_2', t) G_p(R_1', R_2', \lambda') \tag{10}$$

If at any given time only two particles merge, the total possible number of coalesce events is $1/2\, N_v$. The particle collide a rate is then given by $1/2\, N_v \Gamma(R_1,R_2,\lambda) f_c(R_1',R_2',\lambda') dR_1' dR_2' d\lambda'$, where $\Gamma(R_1,R_2,\lambda)$ is the frequency at which two particles R_1 and R_2 initially a distance λ apart coalesce. Integrating over all possible values of R_1,R_2 and λ, the rate of coalescence is given by

$$\dot{N}_v^+(t) = \frac{1}{2} N_v(t) \int_0^\infty \int_0^\infty \int_0^\infty \Gamma(R_1', R_2', \lambda') f_c(R_1', R_2', \lambda') dR_2'\, d\lambda'\, dR_1' \tag{11}$$