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1990 J. Phys.: Condens. Matter 2 6275

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## Many-body effects on the coarsening of grain boundary precipitates

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Received 15 January 1990

**Abstract.** We study the asymptotic behaviour of a diffusion-controlled coarsening of grain boundary precipitates. Using an analogy to two-dimensional particle coarsening, we consider cooperative effects among precipitates occurring via the diffusion field. We discuss the finite volume fraction effects on the form of the precipitate size distribution function and the coarsening rate.

The diffusion-controlled coarsening behaviour of precipitates situated on high-angle grain boundaries has first been studied by Speight and Kirchner (SK) [1]. In this coarsening process the transport of matter from the smaller to the larger precipitates occurs through a two-dimensional intervening medium, that is, grain boundaries. Solving a cylindrically symmetric two-dimensional diffusion equation for solute atoms, they have obtained the  $t^{1/4}$ -growth law of the average precipitate size and the asymptotic steady-state distribution function for precipitate size. They have, however, ignored the many-body effects among precipitates via the diffusion field, which has been shown to play important roles in two- [2–4] and three-dimensional [5] particle coarsening, and in dislocation loop coarsening [6]. Thus, in the present paper, we study such effects on this phenomenon by using an analogy to two-dimensional particle coarsening [2]. In the following discussion, we assume that: (i) the equilibrium precipitate shape is a hemispherical cap of radius  $R$  symmetrically situated with respect to the boundary plane, as used by SK [1]; (ii) the assumption of local equilibrium at the precipitate surface is valid. Different types of boundary conditions will be discussed elsewhere; and (iii) the radius  $R$  is sufficiently larger than the capillary length  $\alpha$ , which is defined below.

To obtain the growth equation of a precipitate we must solve the two-dimensional diffusion equation for the concentration field of solute atoms  $C(\mathbf{r}, t)$ :

$$\frac{\partial}{\partial t} C(\mathbf{r}, t) = D \nabla^2 C(\mathbf{r}, t) \quad (1)$$

with boundary conditions

$$C(\mathbf{r}, t) \rightarrow \bar{C}(t) \quad \text{as } |\mathbf{r}| \rightarrow \infty \quad (2)$$

$$C(\mathbf{r}, t) = C_{\text{eq}}(R) \quad \text{at the precipitate surface.} \quad (3)$$

Here  $D$  is the diffusion coefficient of solute atoms,  $\bar{C}(t)$  the bulk concentration at time

$t$ , and  $C_{\text{eq}}(R)$  the local equilibrium concentration associated with a precipitate of radius  $R$  given by (the Gibbs–Thomson relation)

$$C_{\text{eq}}(R) = C_e \exp(\alpha/R) \approx C_e(1 + \alpha/R) \quad (4)$$

where  $C_e$  is the equilibrium concentration associated with  $R = \infty$ . Moreover,  $\alpha$  is the capillary length and is defined by  $\alpha \equiv 2\gamma v/k_B T$  where  $\gamma$  is the surface energy per unit area of the precipitate-matrix interface,  $v$  is the atomic volume of a solute atom, and  $k_B T$  is the usual thermal energy. The steady-state solution of the above diffusion equation is

$$C(r) = C_1 + C_2 \log|r| \quad (5)$$

with constants  $C_1$  and  $C_2$ , and thus the boundary condition at infinity (2) cannot be satisfied. To resolve this problem, SK have introduced a cut-off distance which serves phenomenologically as an outer limit at which (2) is satisfied. Developing this *ad hoc* technique, Ardell has discussed many-body effects on this coarsening [7].

A similar situation occurs in two-dimensional particle coarsening [2–4]. Recently, using a statistical mechanical method [8], Hayakawa and Family have proved the existence of the screening length within which precipitates are correlated and have determined it self-consistently [4]. Applying a similar analysis to the present phenomenon, we have obtained the growth equation of a hemispherical precipitate with radius  $R$  as [9]

$$2\pi A(d/dt)R^3 = 2\pi wD(R/L(t))G(R/L(t))(\bar{C}(t) - C_{\text{eq}}(R)) \quad (6)$$

with

$$G(x) \equiv K_1(x)/K_0(x) \quad (7)$$

where  $A$  is a geometrical constant defined by SK,  $w$  is the width of the grain boundary,  $L(t)$  the screening length defined below in (11), and  $K_0$  and  $K_1$  are modified Bessel functions. Thus, the growth velocity can be written as

$$(d/dt)R = gG(R/L(t))(R/R_c(t) - 1)/(L(t)R^2) \quad (8)$$

$$g \equiv \alpha wDC_e/3A \quad (9)$$

where  $R_c(t)$  denotes the critical radius given by

$$R_c(t) = \alpha C_e/(\bar{C}(t) - C_e) \quad (10)$$

and is determined later from the mass conservation law. We should remark that in this case, the left hand side of (6) denotes the precipitate volume change, instead of the area change in two-dimensional particle coarsening [2–4]. Accordingly, a self-consistent definition of  $L(t)$  for a small precipitate volume fraction is altered as [9]

$$2\pi AL(t)^3 n(t) = K_1(\bar{R}(t)/L(t)). \quad (11)$$

Here  $n(t)$  is the number density of precipitates defined by

$$n(t) \equiv \int_0^\infty F(R, t) dR$$

and  $\bar{R}(t)$  is the average radius defined by

$$\bar{R}(t) \equiv \int_0^\infty RF(R, t) dR/n(t)$$

where  $F(R, t)$  denotes the precipitate size distribution function per unit volume.

We assume that the distribution function  $F(R, t)$  changes only by the growth or dissolution of precipitates. Thus, it obeys a continuity equation in  $R$ -space:

$$(\partial/\partial t)F(R, t) + (\partial/\partial R)[(dR/dt)F(R, t)] = 0. \tag{12}$$

The bulk concentration  $\bar{C}(t)$  or the critical radius  $R_c(t)$  are constrained by mass conservation:

$$\bar{C}(t) = C_{in} - 2\pi A \int_0^\infty R^3 F(R, t) dR \tag{13}$$

where  $C_{in}$  is the initial concentration.

Now we discuss the asymptotic properties of this coarsening. Equations (8)–(13) are formally analogous to those of [2]. Hence, we should quote only the final results omitting intermediate calculations. In general, the asymptotic form of the distribution is given by

$$F(R, t) \equiv (n(t)/\bar{R}(t))h(x) \tag{14}$$

where  $x$  is a relative precipitate radius defined by  $x \equiv R/\bar{R}(t)$ , and  $h(x)$  denotes a relative size distribution function and is time-independent, satisfying a normalisation

$$\int_0^\infty h(x) dx = 1.$$

The time-dependent behaviour of the system is described by

$$(\bar{R}(t))^4 - (\bar{R}(0))^4 = (3/4)^3 gK(Q)t \tag{15}$$

$$n(t) = (Q/2\pi Am_3)(\bar{R}(t))^{-3} \tag{16}$$

$$F(R, t) = (Q/2\pi Am_3)h(x)(\bar{R}(t))^{-4} \tag{17}$$

where  $\bar{R}(0)$  is the initial average radius,  $K(Q)$  the coarsening rate determined below in (20), and  $m_3$  the third moment defined by

$$m_3 = \int_0^\infty x^3 h(x) dx.$$

From these results the present temporal power laws are found to be identical to those of the SK theory. On the other hand, we obtain  $h(x)$  as

$$h(x) = \begin{cases} (N/I(x, K)) \exp\left(\int_0^x I(y, K)^{-1} dy\right) & \text{for } x < x_0 \\ 0 & \text{for } x \geq x_0 \end{cases} \tag{18}$$

with

$$I(x, K) = (4/3)^4 G(x/s)(x/a - 1)/(K(Q)sx^2) - x/3 \tag{19}$$

where the constant  $N$  is determined by

$$\int_0^\infty h(x) dx = 1$$

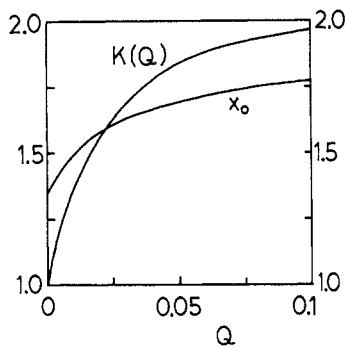
and the coarsening rate  $K(Q)$  and the cut-off  $x_0$  are determined, respectively, by

$$I(x, K) = (d/dx)I(x, K) = 0 \quad \text{for } x = x_0. \tag{20}$$

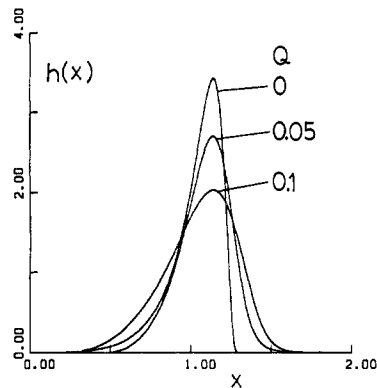
In the long-time limit, two quantities,  $a \equiv R_c(t)/\bar{R}(t)$  and  $s \equiv L(t)/\bar{R}(t)$  in (19) become time-independent, and are defined, respectively, by

$$a = \int_0^\infty xG(x/s)h(x) dx / \int_0^\infty G(x/s)h(x) dx \tag{21}$$

$$s^3/K_1(1/s) = Q/m_3. \tag{22}$$



**Figure 1.** Coarsening rate  $K(Q)$  and cut-off  $x_0$  as a function of the volume fraction  $Q$ .



**Figure 2.** Relative precipitate size distribution function  $h(x)$  versus  $x \equiv R/\bar{R}(t)$  for  $Q = 0$  (the sk theory), 0.05 and 0.1.

These quantities and the third moment  $m_3$  must be determined self-consistently for each value of  $Q$ . We should remark that in the present theory the radius  $R$  is scaled by the average radius  $\bar{R}(t)$ , whereas in the sk theory  $R$  is scaled by the critical radius  $R_c(t)$  with  $R_c(t) = a\bar{R}(t)$ . In the dilute limit  $Q \rightarrow 0$ , we have numerically checked that the present result approaches that of the sk theory. Numerical results for  $K(Q)$ ,  $x_0$  and  $h(x)$  are shown as a function of  $Q$  in figures 1 and 2, respectively.

In summary, we have studied many-body effects on the coarsening of grain boundary precipitates by using an analogy to two-dimensional particle coarsening. Such effects are not found to alter the qualitative behaviour of the temporal power laws. However, with increasing precipitate volume fraction,  $Q$ , the coarsening rate  $K(Q)$  increases and the relative precipitate radius distribution function,  $h(x)$ , broadens. We should remark that even if  $Q$  is small, the dependence on  $Q$  of  $K(Q)$  and  $h(x)$  is remarkable. Comparisons of the present results with those of experiments and with the Ardell theory will be discussed in the future.

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