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RESEARCH ARTICLE

Diffusion-controlled phase growth on dislocations

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We treat the problem of diffusion of solute atoms around screw dislocations. In particular, we express and solve the diffusion equation in 2-dimensions with radial symmetry in an elastic field of a screw dislocation subject to conservation of flux at the interface of a new phase. We consider an incoherent second-phase precipitate growing under the action of the stress field of a screw dislocation. The second-phase growth rate as a function of the supersaturation and a strain energy parameter is evaluated in spatial dimensions $d = 2$. Our calculations show that an increase in the amplitude of dislocation force, e.g. the magnitude of the Burgers vector, enhances the second-phase growth in an alloy. Moreover, we calculate reduction in concentration of solute atoms as a function of radius around a second-phase which grows cylindrically (radial direction) so that its radius varies as a square root of time for various levels of the dislocation force amplitude.

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1. Introduction

Dislocations can alter different stages of the precipitation process in crystalline solids, which consists of nucleation, growth and coarsening [1, 2]. Distortion of the lattice in proximity of a dislocation can enhance nucleation in several ways [3, 4]. The main effect is the reduction in the volume strain energy associated with the phase transformation. Nucleation on dislocations can also be helped by solute segregation which raises the local concentration of the solute in the vicinity of a dislocation, caused by migration of solutes toward the dislocation, the Cottrell atmosphere effect. When the Cottrell atmosphere becomes supersaturated, nucleation of a new phase may occur followed by growth of nucleus. Moreover, dislocation can aid the growth of an embryo beyond its critical size by providing a diffusion passage with a lower activation energy.

Precipitation of second-phase along dislocation lines has been observed in a number of alloys [5, 6]. For example, in Al-Zn-Mg alloys, dislocations not only induce and enhance nucleation and growth of the coherent second-phase $MgZn_2$ precipitates, but also produce a spatial precipitate size gradient around them [7–9]. Cahn [10] provided the first quantitative model for nucleation of second-phase on dislocations in solids. In Cahn's model, it is assumed that a cross-section of the nucleus is circular, which is strictly valid for a screw dislocation [1]. Also, it is posited that the nucleus is incoherent with the matrix so that a constant interfacial energy can be allotted to the boundary between the new phase and the matrix. An incoherent particle interface with the matrix has a different atomic configuration than that

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of the phases. The matrix is an isotropic elastic material and the formation of the precipitate releases the elastic energy initially stored in its volume. Moreover, the matrix energy is assumed to remain constant by precipitation. In this model, besides the usual volume and surface energy terms in the expression for the total free energy of formation of a nucleus of a given size, there is a term representing the strain energy of the dislocation in the region currently occupied by the new phase. Cahn's model predicts that both a larger Burgers vector and a more negative chemical free energy change between the precipitate and the matrix induce higher nucleation rates, in agreement with experiment [5, 6].

Segregation phenomenon around dislocations, i.e. the Cottrell atmosphere effect, has been observed among others in Fe-Al alloys doped with boron atoms [11] and in silicon containing arsenic impurities [12], in qualitative agreement with Cottrell and Bilby's predictions [13]. Cottrell and Bilby considered segregation of impurities to straight-edge dislocations with the Coulomb-like interaction potential of the form $\phi = A \sin\theta / r$, where A contains the elasticity constants and the Burgers vector, and (r, θ) are the polar coordinates. Cottrell and Bilby ignored the flow due concentration gradients and solved the simplified diffusion equation in the presence of the aforementioned potential field. The model predicts that the total number of impurity atoms removed from solution to the dislocation increases with time t according to $N(t) \sim t^{2/3}$, which is in good agreement with the early stages of segregation of impurities to dislocations, e.g. in iron containing carbon and nitrogen [14]. A critical review of the Bilby-Cottrell model, its shortcomings and its improvements are given in [15].

The object of our present study is the diffusion-controlled growth of a new phase, i.e., a post nucleation process in the presence of dislocation field rather than the segregation effect. As in Cahn's nucleation model [10], we consider an incoherent second-phase precipitate growing under the action of a screw dislocation field. This entails that the stress field due to dislocation is pure shear. The equations used for diffusion-controlled growth are radially symmetric. These equations for second-phase in a solid or from a supercooled liquid have been, in the absence of an external field, solved by Frank [16] and discussed by Carslaw and Jaeger [17]. The exact analytical solutions of the equations and their various approximations thereof have been systematized and evaluated by Aaron et al. [18], which included the relations for growth of planar precipitates. Applications of these solutions to materials can be found in many publications, e.g. more recent papers on growth of quasi-crystalline phase in Zr-base metallic glasses [19] and growth of Laves phase in Zircaloy [20]. We should also mention another theoretical approach to the problem of nucleation and growth of an incoherent second-phase particle in the presence of dislocation field [21]. Sundar and Hoyt [21] introduced the dislocation field, as in Cahn [10], in the nucleation part of the model, while for the growth part the steady-state solution of the concentration field (Laplace equation) for elliptical particles was utilized.

The organization of this paper as follows. The formulation of the problem, the governing equation and the formal solution are given in section 2. Solutions of specific cases are presented in section 3, where the supersaturation as a function of the growth coefficient is evaluated as well as the spatial variation of the concentration field in the presence of dislocation. In section 4, besides a brief discourse on the issue of interaction between point defects and dislocations, we calculate the size-dependence of the concentration at the curved precipitate/matrix for the problem under consideration. We have carried out our calculations in space dimensions $d = 2$ corresponding to growth of a second-phase cylinder in radial direction. Some mathematical analyses are relegated to appendix A.

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2. Formulation and general solutions

We consider the problem of growth of the new phase, with radial symmetry (radius r), governed by the diffusion of a single entity, $u \equiv u(r,t)$, which is a function of space and time (r,t). u can be either matter (solvent or solute) or heat (the latent heat of formation of new phase). The diffusion in the presence of an external field obeys the Smoluchowski equation [22] of the form

$$\frac{\partial u}{\partial t} = -\nabla \cdot \mathbf{J}, \tag{1}$$

$$\mathbf{J} = -D(\nabla u - \beta \mathbf{F} u), \tag{2}$$

where D is the diffusivity, $\beta = 1/k_B T$, k_B the Boltzmann constant, T the temperature, and $\mathbf{F}$ is an external field of force. The force can be local (e.g., stresses due to dislocation cores in crystalline solids) or caused externally by an applied field (e.g., electric field acting on charged particles). If the acting force is conservative, it can be obtained from a potential ϕ through $\mathbf{F} = -\nabla\phi$. The considered geometric condition applies to the case of second-phase particles growing in a solid solution under phase transformation [20] or droplets growing either from vapour or from a second liquid [16]. A steady state is reached when $\mathbf{J} = \text{const.} = 0$, resulting in $u = u_0 \exp(-\beta\phi)$.

Combining equations (1) and (2) and expressing it in terms of the potential field ϕ, we write

$$\frac{\partial u}{\partial t} = D(\nabla^2 u + \beta u \nabla^2 \phi + \beta \nabla u \cdot \nabla \phi). \tag{3}$$

Let us suppose, for the sake of a generality, a topological defect in a medium with a potential energy in the form

$$\phi = A r^{\delta} \ln \frac{r}{r_0}, \qquad \text{for} \quad r \geq r_0, \tag{4}$$

where r is a distance, δ a topological exponent, r_0 the defect core size, and A a medium dependent constant. Putting $\delta = d - n$, where d is the spatial dimensionality and n an integer $n \leq d$, then equation (4) with $d = 2$ and $n = 2$ represents the dislocation elastic energy in a crystalline plane or vortex-antivortex pair energy in condensed matter [23], and $d = 3$, $n = 2$ the vortex ring energy in a Bose liquid [24], to give a few examples. Curiously, $\delta = 1$ gives the grain boundary energy in a polycrystalline, where r stands for the spacing of a wall of edge dislocations [25].

Substituting for ϕ from equation (4) with $\delta = d-2$, equation (3) in a rotationally symmetric system can be written in the form

$$\frac{1}{D}\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial r^2} + \Big[\frac{d-1}{r} + \beta A r^{d-3}\Big(1 + (d-2)\ln\big(\frac{r}{r_0}\big)\Big)\Big]\frac{\partial u}{\partial r} + \\ + \beta A (d-2) r^{d-4}\Big[3 + 2(d-2)\ln\big(\frac{r}{r_0}\big)\Big]u, \tag{5}$$

with the boundary conditions $u(r=\infty) = u_m$ and $u(r=R) = u_s$ for $d \geq 2$, where u_m is the mean (far-field) solute concentration in the matrix, u_s is the concentration in the matrix at the new-phase/matrix interface determined from thermodynamics of new phase, i.e., phase equilibrium and the capillary effect, and R is the radius of a platelet in a $d = 2$ setting or the radius of spherical particle in case of $d = 3$.

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Moreover, the conservation of flux at the interface radius R gives

$$K_d R^{d-1} |\mathbf{J}|_{r=R} = q \frac{\mathrm{d}V_d}{\mathrm{d}t}, \tag{6}$$

where $K_d = 2\pi^{d/2}/\Gamma(d/2)$, $\Gamma(x)$ the usual Γ-function, $V_d = 2\pi^{d/2} R^d / d\Gamma(d/2)$, and q the amount of the diffusing entity ejected at the boundary of the growing phase per unit volume of the latter (new phase) formed.

We consider the case $d = 2$ when $A \neq 0$ and assume that the diffusion is toward the core of dislocation line. Also, we suppose that a cross-section of the precipitate (nucleus) perpendicular to the dislocation is circular, i.e., the precipitate surrounds the dislocation. Furthermore, we treat the matrix and solution as linear elastic isotropic media. The elastic potential energy of a stationary dislocation of length l is then given by $\phi = A \ln(r/r_0)$, where $A = Gb^2 l/4\pi$ for screw dislocation, G is the elastic shear modulus of the crystal, b the magnitude of the Burgers vector, ν Poisson's ratio, and r_0 is the usual effective core radius. Also, we assume that the dislocation's elastic energy is relaxed within the volume occupied by the precipitate and that the precipitate is incoherent with the matrix. Hence the interaction energy between the elastic field of the screw dislocation and the elastic field of the solute is zero. In the case of an edge dislocation and coherent precipitate/matrix interface, this interaction is non-negligible. In our reatment, we have tacitly assumed that the molar volume of the second-phase is equal to that of the matrix phase.

Hence, for $d = 2$ (cylindrical symmetry) equation (5) is considerably simplified, namely

$$\frac{1}{D}\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial r^2} + (1+B)\frac{1}{r}\frac{\partial u}{\partial r}. \tag{7}$$

where $B \equiv \beta A$. Now making a usual change of variable to the dimensionless reduced radius $s = r/\sqrt{Dt}$, the partial differential equation (7) is reduced to an ordinary differential equation of the form

$$\frac{\mathrm{d}^2 u}{\mathrm{d}s^2} + \left(\frac{s}{2} + \frac{1+B}{s}\right)\frac{\mathrm{d}u}{\mathrm{d}s} = 0, \tag{8}$$

with the boundary conditions, $u(s=\infty) = u_m$, and $u(s = 2\lambda) = u_s$.

In s-space, the flux conservation equation (6) with $R = 2\lambda\sqrt{Dt}$ is written as

$$\left(\frac{\mathrm{d}u}{\mathrm{d}s}\right)_{s=2\lambda} = -\left(\frac{Bu_s}{2\lambda} + q\lambda\right). \tag{9}$$

The boundary condition $u(2\lambda) = u_s$ and equation (9) will provide a relationship between u_s and u_m through λ.

The diffusion problem considered here describes the growth of cylinder (circular plate) on a dislocation line. We note that the present model does not account for the fast diffusion of atoms along the dislocation line. Diffusion of atoms takes place only in the matrix and the diffusion coefficient D can be considered as the bulk diffusivity. So, when the atoms reach the dislocation core they precipitate and grow according to $R = 2\lambda\sqrt{Dt}$. Our aim is to calculate λ as a function supersaturation for various values of the dislocation force amplitude (see the next section).

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Equation (8) has a general solution in the form

$$u(s) = u_m + \frac{(Bu_m + 2q\lambda^2)\lambda^B e^{\lambda^2}\Gamma(-B/2, s^2/4)}{2 - B\lambda^B e^{\lambda^2}\Gamma(-B/2, \lambda^2)}, \tag{10}$$

where we utilized $u(\infty) = u_m$ and equation (9). Here $\Gamma(a, z)$ is the incomplete gamma function defined by the integral $\Gamma(a, z) = \int_z^\infty t^{a-1}e^{-t}dt$ [26]. The yet unknown parameter λ is found from relation (10) at $u(2\lambda) = u_s$ for a set of input parameters u_s, u_m q, and B, through which the concentration field, equation (10), and the growth of second-phase particle are determined. Note that our problem formulation supposes that at time $t = 0$, the particle radius is zero. In addition, the capillarity of the second-phase is neglected, both in the boundary conditions and in equation (9) as in the free diffusion case treated in [16, 18].

3. Computations

To study the growth behavior of a second-phase in a solid solution under the action of screw dislocation field, we attempt to compute the growth rate constant as a function of the supersaturation parameter k, defined as $k \equiv (u_s - u_m)/q$ with $q = u_p - u_s$, where u_p is the composition of the nucleus [18]. Equation (10) with $u(2\lambda) = u_s$ yields

$$k = \left[\frac{2\lambda^2 + Bu_m(u_p - u_s)^{-1}}{2 - B\lambda^B e^{\lambda^2}\Gamma\big(-B/2, \lambda^2\big)}\right]\lambda^B e^{\lambda^2}\Gamma\big(-B/2, \lambda^2\big). \tag{11}$$

For $B = 0$, the relations obtained by Frank [16] are recovered, namely

$$u(z) = u_m + q\lambda^2 e^{\lambda^2} E_1(z^2/4), \tag{12}$$

$$k = \lambda^2 e^{\lambda^2} E_1(\lambda^2), \tag{13}$$

where $E_1(x)$ is the exponential integral of order one, related to the incomplete gamma function through the identity $E_n(x) = x^{n-1}\Gamma(1 - n, x)$; and $E_1(x) = -\mathrm{Ei}(-x)$, where $\mathrm{Ei}(x) = -\int_{-x}^\infty e^{-t}t^{-1}dt$ [26].

From equation (11), it is seen that a complete separation of the supersaturation parameter $k \equiv (u_s - u_m)(u_p - u_s)^{-1}$ is not possible for $B \neq 0$. However, for $u_s << u_p$ (a reasonable proviso) we write

$$k = \left[\lambda^2 + \frac{B}{2}\left(\epsilon + \mathcal{O}(\epsilon^2)\right)\right]\lambda^B e^{\lambda^2}\Gamma\big(-B/2, \lambda^2\big), \tag{14}$$

with $\epsilon \equiv u_s/u_p$. We can then calculate the spatial variation of the concentration as a function of the amplitude of the dislocation force B and the growth coefficient λ (cf. appendix A). For $B = 1$, equations (10) and (14) yield, respectively

$$u(z) = u_m + \frac{2\lambda\, e^{\lambda^2}\,(u_m + 2q\lambda^2)\, E_{3/2}(z^2/4)}{[2 - e^{\lambda^2}E_{3/2}(\lambda^2)]z}, \tag{15}$$

$$k = \left(\lambda^2 + \frac{\epsilon}{2}\right) e^{\lambda^2} E_{3/2}(\lambda^2) + \mathcal{O}(\epsilon^2). \tag{16}$$

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Similarly for $B = 2$, we have

$$u(z) = u_m + \frac{4\lambda^2 e^{\lambda^2}(u_m + q\lambda^2)E_2(z^2/4)}{[1 - e^{\lambda^2}E_2(\lambda^2)]z^2}, \tag{17}$$

$$k = (\lambda^2 + \epsilon)E_2(\lambda^2) + \mathcal{O}(\epsilon^2). \tag{18}$$

We have plotted the growth coefficient $\lambda = R/(2\sqrt{Dt})$ as a function of the supersaturation parameter k in figure 1 and the spatial variation of the concentration field in figure 2 for several values of B. The computations are performed to $\mathcal{O}(\epsilon^2)$ with $\epsilon = 0.01$. Figure 1 shows that λ is an increasing function of k; and also, as B is raised λ is elevated. This means that an increase in the amplitude of dislocation force (e.g., the magnitude of the Burgers vector) enhances second-phase growth in an alloy.

Figure 2 displays the reduced concentration versus the reduced radius $z = r/\sqrt{Dt}$ for $\lambda = 1$. The reduced concentration is calculated via equation (10). The curves in figure 2 show decrease in concentration as a function distance around a new phase growing cylindrically so that its radius R is proportional to $t^{1/2}$, when $\lambda = R/(2\sqrt{Dt}) = 1$. For the sake of precision, a few data points from these plots are listed in table 1. Our results for $B = 0$ match those obtained by Frank [16]. It is seen that for $z \lesssim 1.6$ the concentration is enriched with increase in B, whereas for $z \gtrsim 1.6$, it is vice versa. So, for $\lambda = 1$, the crossover z-value is $z_c \approx 1.6$. Also, as λ is reduced, z_c is decreased. Large and small z behaviours of $u(z)$ are calculated in appendix A.

Table 1. Reduced concentration vs. distance z at several values of the force amplitude B and at $\lambda = 1$, cf. figure 2. Computations were carried out up to and including $\mathcal{O}(\epsilon^2)$ with $\epsilon = 0.01$.

z	$B = 0$	$B = 1$	$B = 2$	$B = 3$	$B = 4$
0.5	6.1349	13.5233	35.0732	101.4977	315.7501
1	2.8387	3.8669	5.6862	8.8579	14.4066
1.5	1.3333	1.3537	1.4346	1.5731	1.7725
2	0.5963	0.4867	0.4077	0.349	0.3042
2.5	0.2479	0.1696	0.118	0.0833	0.0595
3	0.0945	0.0557	0.0332	0.02	0.0121
3.5	0.0328	0.017	0.0088	0.0046	0.0025
4	0.0103	0.0047	0.0022	0.001	0.0005

4. Discussion

The potential energy in equation (4) with $\delta = 0$ describes the elastic energy of the dislocation relaxed within the volume occupied by the second-phase precipitate [10]. It was treated here as an external field affecting the diffusion-limited growth of second-phase precipitate. The interaction energy of impurities in a crystalline with dislocations depends on the specific model or configuration of a solute atom and a matrix which is used. Commonly, it is assumed that the solute acts as an elastic center of dilatation. It is a fictitious sphere of radius R' embedded concentrically in a spherical hole of radius R cut in the matrix. If the elastic constants of the solute and matrix are the same, the work done in inserting the atom in the presence of dislocation is $w = p\Delta v$, where p is the hydrostatic pressure and Δv is the difference between the volume of the hole in the matrix and the sphere of the fictitious impurity. For a screw dislocation $p = 0$, while near an edge dislocation

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$p = \frac{(1+\nu)bG\sin\theta}{3\pi(1-\nu)r}$ for an impurity with polar coordinates (r, θ) with respect to the dislocation $0z$, hence $w \propto \Delta v \sin\theta/r$ [13]. Using a nonlinear elastic theory [27], a screw dislocation may also interact with the spherical impurity with the interaction energy $w \propto \Delta v/r^2$. Moreover, accounting for the differences in the elastic constants of a solute and a matrix, the solute will relieve shear strain energy as well as dilatation energy, which will also interact with a screw dislocation with a potential $w \propto \Delta v/r^2$ [28]. Indeed, Friedel [28] has formulated that by introducing a dislocation into a solid solution of uniform concentration c_0, the interaction energy between the dislocation and solute atoms can be written as $w \backsimeq w_0(b/\rho)^n f(\theta)$, where ρ is the distance between the two defects, w_0 the binding energy when $\rho = b$, and $f(\theta)$ accounts for the angular dependence of the interaction along the dislocation. Also, $n = 1$ for size effects and $n = 2$ for effects due to differences in elastic constants. The discussed model for the interaction energy between solute atoms and dislocations has been used to study the precipitation process on dislocations by number of workers in the past [29, 30] and thoroughly reviewed in [15]. These studies concern primarily the overall phase transformation (precipitation of a new phase) rather than the growth of a new phase considered in our note. That is, they used different boundary conditions as compared to the ones used here.

As alluded in section 1, the solute-dislocation potential energy of the form A/r in the diffusion equation, during the early stages of segregation, would predict that the Cottrell cloud solute number evolves as $N \sim t^{2/3}$, and consequently its radius as $R \sim t^{1/3}$ [15]. Our calculations deal with the growth of circular plate according to $R \sim t^{1/2}$. Hin et al.'s investigations [31, 32] utilizing this kind of potential (A/r) and a kinetic Monte Carlo simulation in three dimensions, qualitatively indicate that at the beginning of an isothermal-annealing experiment, e.g. on the Fe-C system, the radius of the Cottrell cloud grows roughly as $\sim t^{1/3}$, during which small ovoid precipitates nucleate. After some lapse of time, the ovoid particles grow lengthwise along the dislocation line and coalesce, completely wetting the dislocation line by forming a cylindrical shaped precipitate [31]. Then the radius of this cylinder is expected to grow parabolically with time, $R \sim t^{1/2}$. Our calculations may be pertinent to this stage of precipitate evolution. Hin et al.'s simulations show that at much longer times, the precipitate de-wets the dislocation re-forming to ovoid particles.

Let us now link the supersaturation parameter k to an experimental situation. For this purpose, the values of u_s, i.e. the concentration at the interface between the second-phase and matrix should be known. The capillarity effect leads to a relationship between u_s and the equilibrium composition u_{eq} (solubility line in a phase diagram). To obtain this relationship, we consider an incoherent nucleation of second-phase on a dislocation à la Cahn [10]. A Burgers loop around the dislocation in the matrix material around the incoherent second-phase (circular plate) will have a closure mismatch equal to b. Following Cahn, on forming the incoherent plate of radius R, the total free energy change per unit length is

$$\mathcal{G} = -\pi R^2 \Delta g_v + 2\pi\gamma R - A' \ln(R/r_0), \tag{19}$$

where Δg_v is the volume free energy of formation, γ the interfacial energy and the last term is the dislocation energy, $A' = Gb^2/4\pi$ for screw dislocations. Setting $\mathrm{d}\mathcal{G}/\mathrm{d}R = 0$, yields

$$R = \frac{\gamma}{2\Delta g_v}\left(1 \pm \sqrt{1-\alpha}\right), \tag{20}$$

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where $\alpha = 2A'\Delta g_v/\pi\gamma^2$. So, if $\alpha > 1$, the nucleation is barrierless, i.e., the phase transition kinetics is only governed by growth kinetics, which is the subject of our investigation here. If, however, $\alpha < 1$, there is an energy barrier and the local minimum of $\mathcal{G}$ at $R = R_0$, which corresponds to the negative sign in equation (20), ensued by a maximum at $R = R^*$ corresponding to the positive sign in this equation. The local minimum corresponds to a subcritcal metastable particle of the second-phase surrounding the dislocation line, and it is similar to the Cottrell atmosphere of solute atoms in a segregation problem. When $\alpha = 0$, corresponding to $B = 0$, the two phases are in equilibrium and the maximum in $\mathcal{G}$ is infinite, as for homogeneous nucleation.

For a dilute regular solution, $\Delta g_v = (k_B T/V_p)\ln(u_s/u_{eq})$, where V_p is the atomic volume of the precipitate compound, u_s is the concentration of the matrix at a curved particle/matrix interface and u_{eq} that of a flat interface, which is in equilibrium with the solute concentration in the matrix. Equation (20) gives $\Delta g_v = \gamma/R - A'/2\pi R^2$. Hence, for a dilute regular solution, we write

$$u_s = u_{eq}\exp\Big[\frac{\zeta}{R}\Big(1-\frac{\eta}{R}\Big)\Big], \tag{21}$$

where $\zeta = \beta V_p\gamma$, $\beta = 1/k_B T$ and $\eta = A'/2\pi\gamma$. Subsequently, the supersaturation parameter is expressed by

$$k = \frac{u_{eq}\exp[\frac{\zeta}{R}(1-\frac{\eta}{R})] - u_m}{u_p - u_{eq}\exp[\frac{\zeta}{R}(1-\frac{\eta}{R})]}. \tag{22}$$

Taking the following typical values: $\gamma = 0.2$ Jm^{-2}, $G = 40$ GPa, and $b = 0.25$ nm, then $A' \approx 2.0\times10^{-10}$ N and $\eta = 0.16$ nm. Figure 3 depicts u_s/u_{eq}, from equation (21), as a function of scaled radius R/ζ for $V_p = 1.66\times10^{-29}$ m^3, $\eta = 0$ and $\eta = 0.16$ nm at $T = 600$ K. Equation (21) is analogous to the Gibbs-Thomson-Freundlich relationship [4] comprising a dislocation defect. Recalling now the values used for the interaction parameter B in the computations presented in the foregoing section, we note that for $B = 2$ and the above numerical values for G and b at $T = 1000$ K, we find $l \approx 0.14$ nm, which is close to the calculated value of η.

We should, however, recall that in our problem formulation of the diffusion-controlled growth (section 2), we neglected the capillarity effect of the second-phase, corresponding to $\gamma = 0$, which simplifies equation (21) to

$$u_s = u_{eq}\exp\Big[-\frac{\beta V_p G b^2}{8\pi^2 R^2}\Big]. \tag{23}$$

If now $8\pi^2 R^2 >> \beta V_p G b^2$, or alternatively, $u_s(t\to\infty) = u_{eq}$, equation (22) reduces to

$$k = \frac{u_{eq} - u_m}{u_p - u_{eq}}. \tag{24}$$

In Cahn's model, the assumption that all the strain energy of the dislocation within the volume occupied by the nucleus can be relaxed to zero demands that the nucleus is incoherent. For a coherent nucleus forming on or in proximity of dislocations, this supposition is not true. Instead, it is necessary to calculate the elastic interaction energy between the nucleus and the matrix, which for an edge dislocation is in the form $Gb^2/[4\pi(1-\nu)r]$ for the energy density per unit length [33]. In the same manner, to extend our calculations for growth of coherent precipitate, we must

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employ this kind of potential energy, i.e. the potential energy of the form $\phi(r) = -A\ln(r/r_0) + C\sin\theta/r$, in the governing kinetic equation rather than relation (4).

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Figure captions

Figure 1. Growth coefficient λ as a function of supersaturation k at various levels of dislocation force amplitude B for a circular plate ($d = 2$) and $u_s = 0.01u_p$.

Figure 2. Reduced concentration field as a function of reduced distance from the surface of the circular plate ($d = 2$) at various levels of dislocation force amplitude B and at $\lambda = 1$.

Figure 3. The size dependence of the concentration at the curved precipitate/matrix interface u_s relative to that of the flat interface u_{eq} for a set of parameter values given in the text, cf. eq. (21).

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Appendix A. Evaluation of solution of equation (8)

The general solution of equation (8) subject to the flux conservation relation (6) and the assigned boundary conditions (with $z \equiv s$) can be expressed as

$$u(z) = u_m + qA_2\Gamma\big(-\frac{B}{2}, \frac{z^2}{4}\big) \tag{A1}$$

$$A_2 \equiv \frac{(\frac{B}{2}\frac{u_m}{q} + \lambda^2)\lambda^B e^{\lambda^2}}{1 - \frac{B}{2}\lambda^B e^{\lambda^2}\Gamma(-\frac{B}{2}, \lambda^2)}. \tag{A2}$$

As can be seen, the spatial dependence of the concentration field $u(z)$ is expressed by the incomplete gamma function $\Gamma(-B/2, z^2/4)$, which is a sharply decreasing function z and it tends to zero at large z, resulting $u(z \to \infty) = u_m$. Since $u(2\lambda) = u_s$ and $q = u_p - u_s$, we write

$$\frac{u(z) - u_m}{u_p - u_s} = A_2\Gamma\big(-\frac{B}{2}, \frac{z^2}{4}\big), \tag{A3}$$

For $u_s << u_p$, $\epsilon = u_s/u_p$, and $k = (u_s - u_m)/q$, we find

$$A_2 = \frac{\big[\frac{B}{2}(\epsilon + \mathcal{O}(\epsilon^2) - k) + \lambda^2\big]\lambda^B e^{\lambda^2}}{1 - \frac{B}{2}\lambda^B e^{\lambda^2}\Gamma(-\frac{B}{2}, \lambda^2)}. \tag{A4}$$

Substituting for k from equation (14) in equation (A4) yields

$$A_2 = \big[\frac{B}{2}\big(\epsilon + \mathcal{O}(\epsilon^2)\big) + \lambda^2\big]\lambda^B e^{\lambda^2} \tag{A5}$$

Let us investigate the solution equation (A1) in the limit of small z and large z. For small values of z, series expansion of the incomplete gamma function gives

$$\begin{aligned}\Gamma\big(-\frac{B}{2}, \frac{z^2}{4}\big) = \Gamma\big(-\frac{B}{2}\big) + z^{-B}\big[\frac{2^{B+1}}{B} - \frac{2^{B-1}}{B-2}z^2 + \\ + \frac{2^{B-4}}{B-4}z^4 - \frac{2^{B-6}}{3(B-6)}z^6 + \mathcal{O}(z^8)\big].\end{aligned} \tag{A6}$$

Note that in the limit $B \to 0$, Frank's result is recovered, viz

$$\begin{aligned}\Gamma\big(0, \frac{z^2}{4}\big) = -\gamma + \ln 4 - 2\ln z + \\ + \frac{z^2}{4} - \frac{z^4}{64} + \frac{z^6}{1152} + \mathcal{O}(z^8),\end{aligned} \tag{A7}$$

where γ is Euler's constant. Hence, in this limit, equation (A1) reduces to

$$\frac{u(z) - u_m}{u_p - u_s} = 2\lambda^2 e^{\lambda^2} n_e\big(1 - \frac{1}{n_e}\ln z\big) + \mathcal{O}(z^2), \tag{A8}$$

with $n_e = (-\gamma + \ln 4)/2$.

For large z, we use the asymptotic expansion, and obtain

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$$\Gamma\Big(-\frac{B}{2},\frac{z^2}{4}\Big)=\frac{e^{-\frac{1}{4}z^2}}{z^B}\Big[\frac{4^{B/2+1}}{z^2}-\frac{2^{B+3}(B+2)}{z^4}+ \\ +\frac{2^{B+4}(B^2+6B+8)}{z^6}+\mathcal{O}(\frac{1}{z^7})\Big]. \tag{A9}$$

Hence, for very large z, equation (A1) may be written as

$$\frac{u(z)-u_m}{u_p-u_s}\approx A_2\frac{e^{-\frac{1}{4}z^2}}{z^{B+2}}, \tag{A10}$$

Equation (A10) shows that as z increases, the concentration field $u(z)$ falls rapidly toward u_m for $B\geq 0$.

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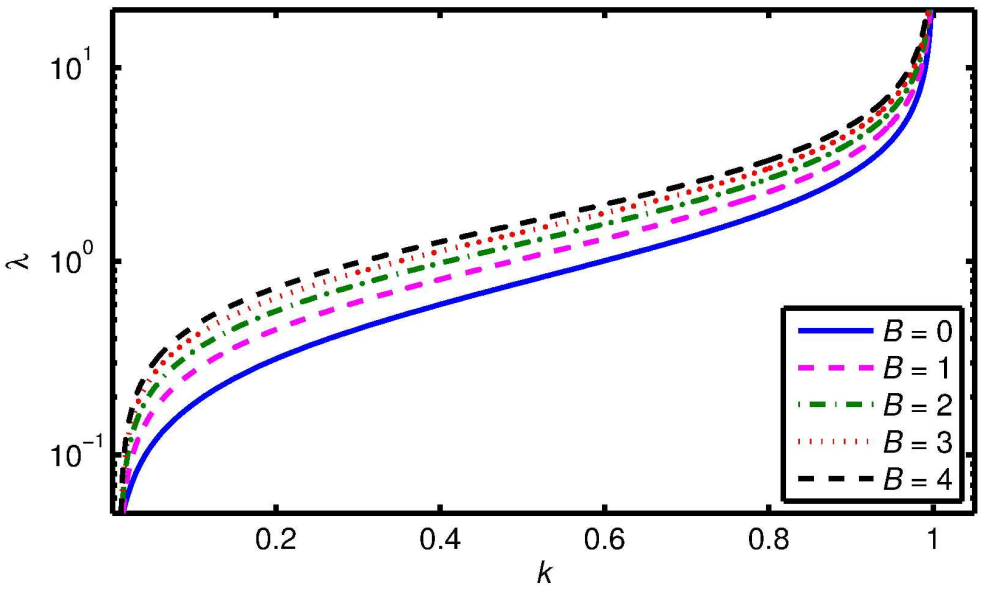

Figure 1
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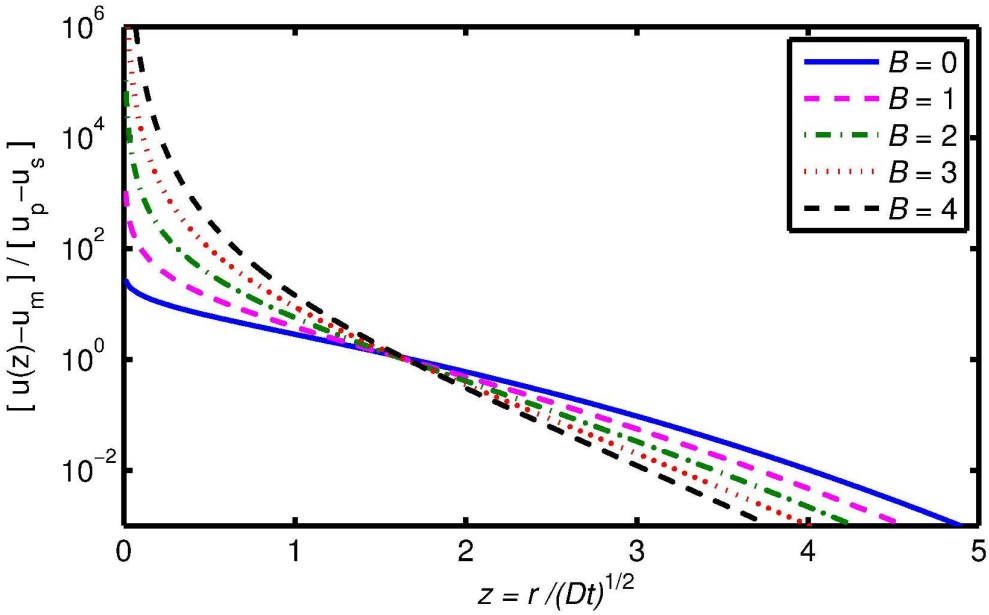

Figure 2
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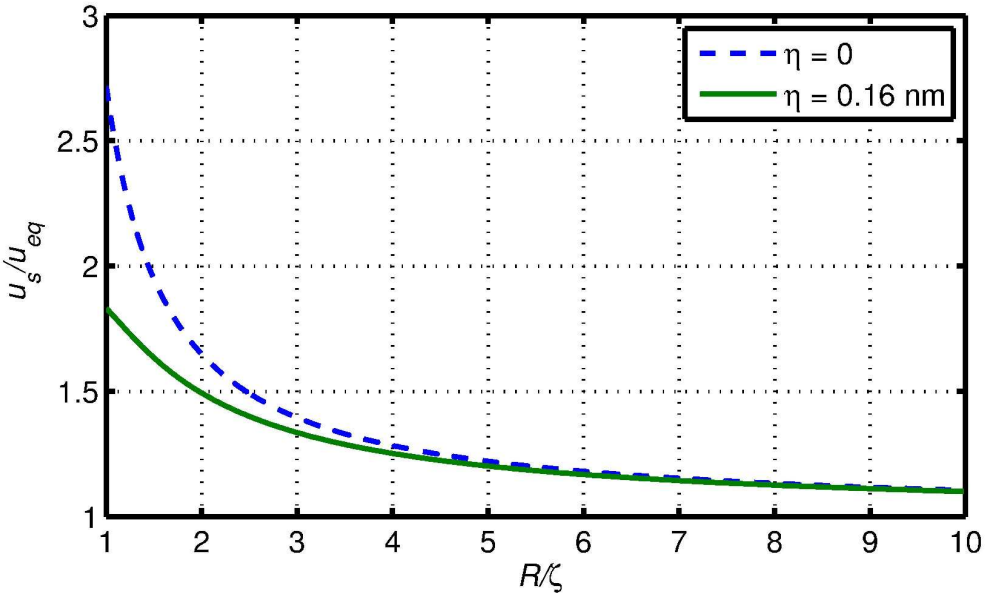

Figure 3
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