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1989 J. Phys.: Condens. Matter 1 9785

(http://iopscience.iop.org/0953-8984/1/48/025)

J. Phys.: Condens. Matter **1** (1989) 9785–9789. Printed in the UK

**LETTER TO THE EDITOR**

# Many-body effects on diffusion-controlled dislocation loop coarsening

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Received 11 September 1989

**Abstract.** We study a diffusion-controlled coarsening process of dislocation loops. Using an analogy to particle coarsening (Ostwald ripening), we consider cooperative effects among loops occurring via the diffusion field. Applying a statistical mechanical method developed by us and our colleagues to this phenomenon, we discuss many-body effects on the form of loop size distribution function and the coarsening rate.

Dislocation loop coarsening has been studied recently by Burton and Speight (BS) [1] using an analogy with particle coarsening [2]. This coarsening process proceeds by the growth of larger loops at the expense of smaller ones, with the total loop area being conserved. BS have, however, ignored the cooperative effects among dislocation loops occurring via the diffusion field, which, as has been pointed out, plays an important role in particle coarsening [3]. To study such effects systematically, we and our colleagues have recently developed a statistical mechanical method [4]. Using this method, we have discussed many-body effects on the asymptotic behaviour of particle coarsening [5]. Thus, in the present letter, we apply this method to dislocation loop coarsening and study such effects on this phenomenon.

We consider a collection of $N$ loops with radii $R_i(t)$ centred at $X_i$. In the following discussion, we assume [1] that (i) the dislocation loop is of vacancy type, completely circular and immobile; (ii) there is no external sink and source, such as a defect in the system: thus, the total loop area is conserved; (iii) the stacking fault energy per unit area is so small as to be negligible; and (iv) the loop radius $R$ is sufficiently large that the exponential term may be expanded in the form $\exp(a/R) \simeq 1 + a/R$, where $a$ is defined in (4) below.

To obtain the growth equation of dislocation loops, we must first solve the diffusion equation for vacancy concentration $C(\boldsymbol{r}, t)$ at position $\boldsymbol{r}$ and time $t$

$$(\partial/\partial t)C(\boldsymbol{r}, t) = D\,\nabla^2 C(\boldsymbol{r}, t) \tag{1}$$

subject to the boundary conditions

$$C(\boldsymbol{r}_i, t) = C_{\mathrm{eq}}(1 + a/R_i) \tag{2}$$

$$C(\boldsymbol{r}, t) \rightarrow \bar{C}(t) \qquad \text{as } |\boldsymbol{r}| \rightarrow \infty \tag{3}$$

with

$$a = b\Omega G/k_{\mathrm{B}}T \tag{4}$$

where $D$ is the vacancy diffusion coefficient, $\boldsymbol{r}_i$ the position vector on the $i$th loop, $C_{\mathrm{eq}}$

the thermal equilibrium concentration, and $\bar{C}(t)$ the average concentration. Here $b$ is the atomic size, $\Omega$ ($\simeq b^3$) the atomic volume, $k_BT$ the thermal energy and $G$ the shear modulus. These equations, with the stationary state approximation $\partial C/\partial t = 0$, have already been solved for particle coarsening by means of a Green function method and provided the growth equation for particles [6]. A similar analysis leads to the growth equation for the $i$th loop:

$$(\mathrm{d}/\mathrm{d}t)\pi R_i^2 = 2\pi\alpha B(i) \tag{5}$$

$$B(i) = R_i/R_c(t) - 1 - R_i \sum_{j\neq i} B(j)/|X_i - X_j| \tag{6}$$

with

$$\alpha = 2b^2 a C_{\mathrm{eq}} D \tag{7}$$

$$R_c(t) = aC_{\mathrm{eq}}/(\bar{C}(t) - C_{\mathrm{eq}}). \tag{8}$$

Here the critical radius $R_c(t)$ is determined from the loop area conservation:

$$\sum_{i=1}^{N(t)} B(i) = 0 \tag{9}$$

where $N(t)$ is the total number of loops at time $t$.

Equation (5), together with equations (6)–(9), is a starting point for studying the coarsening process. This equation consists of two terms. The first two terms in (6) are the mean-field terms, which were discussed by BS. The last term in (6) represents the spatial interaction between loops via the diffusion field. As was pointed out in [4], such systems have two kinds of characteristic length. One is the average loop radius $\bar{R}(t)$. The other is the correlation length, $L(t)$, within which two loops are correlated via the diffusion field, and is defined by

$$L(t) = (2\pi b n(t))^{-1/2} \tag{10}$$

where $n(t)$ is a number density of loops at time $t$. We assume that the number density $n(t)$ is small so that $\bar{R}(t)/L(t) = (2Q/m_2(t))^{1/2} < 1$, where $Q$ is the area fraction defined by $Q = b\pi\Sigma_i R_i^2/V$ where the system volume is $V$, and $m_2(t)$ is the second moment defined by $m_2(t) = \Sigma_i(R_i/\bar{R}(t))^2/N(t)$. Here we note that the area fraction $Q$ is time-independent, from (9). These equations (5)–(9) are formally identical to those for particle coarsening. Thus, the intractable last term in (6) is expected to be renormalised to the first one using the same systematic expansion in powers of $Q^{1/2}$ as in [4].

Now we define the loop size distribution function $F(R, t)$ per unit volume as

$$F(R, t) = V^{-1}\left\langle \sum_i \delta(R - R_i(t)) \right\rangle \tag{11}$$

where $\langle \ldots \rangle$ denotes the average over the initial ensemble. Differentiating $F(R, t)$ with respect to the time $t$ and using (5) leads to the well known BBGKY-like hierarchy equations for the distribution functions. The systematic expansion in powers of $Q^{1/2}$ is then performed, to truncate such hierarchy equations [4]. As a result, we obtain the kinetic equation for $F(R, t)$, up to order $Q^{1/2}$:

$$(\partial/\partial t)F(R, t) + \alpha(\partial/\partial R)(B(x, Q)F(R, t)/R) = 0 \tag{12}$$

with

$$B(x, Q) = x - 1 - (2Q/m_2(t))^{1/2}x(m_2(t) - x) \tag{13}$$

$$m_2(t) = \int_0^\infty (R/\bar{R}(t))^2 F(R, t)\,\mathrm{d}R \Big/ \int_0^\infty F(R, t)\,\mathrm{d}R \tag{14}$$

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

$$\bar{R}(t) = \int_0^\infty RF(R, t)\,\mathrm{d}R \Big/ \int_0^\infty F(R, t)\,\mathrm{d}R.$$

The relative loop radius $x$ is defined by $x = R/\bar{R}(t)$, and the loop number density $n(t)$ is defined by

$$n(t) = \int_0^\infty F(R, t)\,\mathrm{d}R.$$

The first two terms in (13) are the same as those of the BS theory. On the other hand, the last term in (13) denotes the renormalised cooperative effects among loops, which have been studied by none of the previous authors. Further details of the present derivation will be published separately.

Equations (12)–(14) are formally analogous to those of the BS theory and of the particle coarsening [5]. Hence, we shall quote only the final results, omitting intermediate calculations. In general, the asymptotic form of the distribution is given by

$$F(R, t) = (n(t)/\bar{R}(t))h(x) \tag{15}$$

where $h(x)$ is a relative loop size distribution function and is time-independent, satisfying a normalisation condition $\int_0^\infty h(x)\,\mathrm{d}x = 1$. In terms of $h(x)$, the second moment $m_2$ is redefined as $m_2 = \int_0^\infty x^2 h(x)\,\mathrm{d}x$ and thus becomes time-independent. The time-dependent behaviour of the system is described by

$$\bar{R}(t)^2 - \bar{R}(0)^2 = (\alpha/2)K(Q)t \tag{16}$$

$$n(t) = (Q/\pi m_2 b)\bar{R}(t)^{-2} \tag{17}$$

$$F(R, t) = (Q/\pi m_2 b)h(x)\bar{R}(t)^{-3} \tag{18}$$

where $\bar{R}(0)$ is the initial average radius and $K(Q)$ the coarsening rate given by

$$K(Q) = (\sqrt{2Qm_2} - 1)^2 + 4\sqrt{2Q/m_2}. \tag{19}$$

From these results we find that the average loop radius grows as $t^{1/2}$ and the number density of loops decays as $t^{-1}$. These temporal power laws are identical to those of the

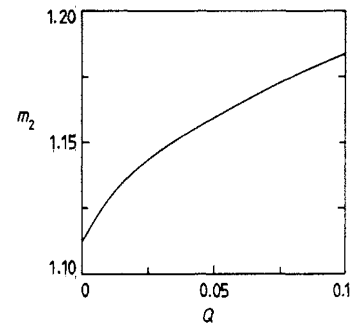


**Figure 1.** The second moment, $m_2$, as a function of the area fraction, $Q$.

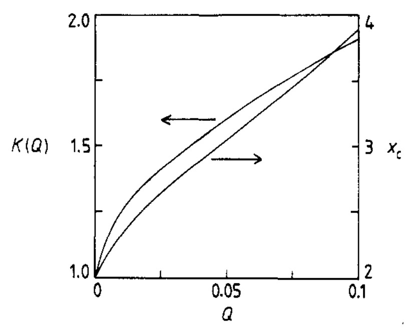


**Figure 2.** The coarsening rate, $K(Q)$, and the cut-off, $x_c$, as a function of the area fraction, $Q$.

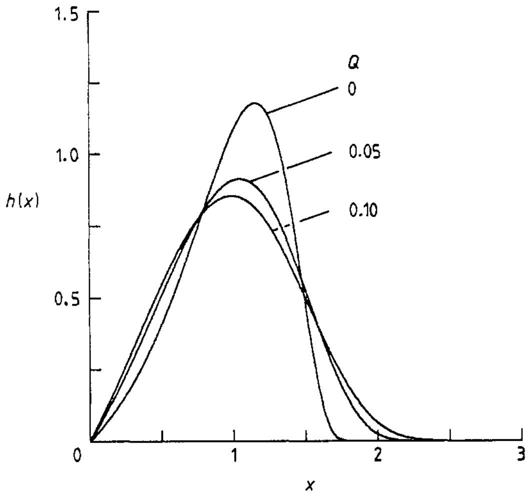


**Figure 3.** The relative loop size distribution function $h(x)$ against $x = R/\bar{R}$ for $Q = 0$ (the BS theory), 0.05 and 0.1.

BS theory. Thus the many-body effects are not found to alter the qualitative behaviour of the temporal power laws. Finally we obtain the analytic form of $h(x)$:

$$h(x) = \begin{cases} Ax(x_c - x)^{-2-z} \exp[-zx_c/(x_c - x)] & \text{for } x < x_c \\ 0 & \text{for } x \geqslant x_c \end{cases} \tag{20}$$

where the cut-off $x_c$ is given by

$$x_c = 2(1 - \sqrt{2Qm_2})/(K(Q) - 4\sqrt{2Q/m_2}) \tag{21}$$

with $A = zx_c^z \exp(z)$ and $z = 2K(Q)/(K(Q) - 4\sqrt{2Q/m_2})$. Here we should remark that the second moment $m_2$ must be determined self-consistently for each value of $Q$. In the dilute limit $Q \to 0$, we have $K(Q) = 1$ and $x_c = 2$ from (19) and (21), and thus we can recover the BS theory. Numerical results for $m_2$, $x_c$ and $K(Q)$ and $h(x)$ are shown as a function of $Q$ in figures 1–3, respectively.

In summary, we have studied many-body effects among dislocation loops on coarsening by using a systematic method of expansion in powers of $Q^{1/2}$. With increasing area fraction $Q$, the coarsening rate $K(Q)$ increases and the relative loop size distribution function $h(x)$ broadens, while the temporal power laws still hold. These results are similar to those for particle coarsening. We should note that even if $Q$ is small, the dependence on $Q$ of $K(Q)$ and $h(x)$ is remarkable. For reliable studies of loop coarsening we must discuss the effects of the higher-order corrections in the $Q^{1/2}$-expansion as well as the other coarsening mechanism. Such a study is now under way. The results, together with a comparison of the present results with experiment, will be published in the future.

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