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Impurity-concentration profile for an exponentially decaying diffusion coefficient in irradiation enhanced diffusion*

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The diffusion equation is solved for a semi-infinite region in the case of irradiation-enhanced diffusion produced by a diffusion coefficient falling off exponentially in the medium. Near the surface the concentration profile due to enhanced diffusion has a larger concentration than the profile due to thermal diffusion; conversely far from the surface the enhanced-diffusion profile has a lower concentration than that due to thermal diffusion. Thus, this type of enhanced diffusion results in a more abruptly changing profile than does thermal diffusion.

Several mechanisms by which irradiation-enhanced diffusion can occur have been discussed in the literature.[1–4] These include: (i) defect-enhanced diffusion in which diffusion can be enhanced by the presence of defects such as might be created by high-energy bombarding particles; (ii) recoil-enhanced diffusion in which the recoil momentum imparted by a collision between a high-energy particle and a diffusing atom can enhance diffusion; and (iii) ionization-enhanced diffusion. In this latter case there are several mechansims by which ionization can enhance diffusion: (i) the "normal" ionization-enhanced diffusion[4] in which a change in charge-state results in a state of lower migration energy; (ii) the Bourgoin mechanism[5–7] in which the diffusion saddle-point and equilibrium configurations are interchanged between charge states; and (iii) the energy-release mechanism[4] in which the release of strain energy or thermal energy in the vicinity of the defect enhances its diffusion.

The usual experimental configuration for the study of irradiation-enhanced diffusion involves an external beam of particles impinging on the sample. The external beam usually experiences an attenuation in the sample which in turn results in an inhomogeneity in the diffusion enhancement. St. Peters *et al.*[8] considered the concentration profile which resulted from a constant enhanced-diffusion coefficient over a finite sample depth. Here we consider the case of an enhanced diffusivity which decreases exponentially with depth into the sample; such a dependence arises naturally in ionization-enhanced diffusion (either due to the attenuation of an external beam or carriers injected from a junction), but may be approximately correct in defect-enhanced and recoil-enhanced diffusion. We further assume that the temperature is sufficiently low that thermal diffusion is negligible. Then if the assumption of Fickian diffusion is valid for the irradiated sample, the impurity concentration must satisfy

$$\partial_t u = \partial_x (D_r e^{-\beta x} \partial_x u), \tag{1}$$

where $u(x, t)$ is the concentration of impurity atoms, D_r is the value of the irradiation-enhanced-diffusion coefficient at the surface, and $1/\beta$ is the distance from the surface where the intensity of radiation falls off by e^{-1}. The sample is assumed to occupy the region $0 \leq x < \infty$ (i.e., we assume the sample length $L \gg 1/\beta$), and $u(x, t)$ must be bounded as $x \to \infty$. We take the initial and boundary conditions to be

$$\begin{aligned} &u(x, t=0) = 0, \quad x > 0, \\ &u(x=0, t) = u_0, \quad t \geq 0, \end{aligned} \tag{2}$$

corresponding to a thick layer of impurity atoms deposited on the surface of the impurity-free sample prior to the irradiation. The Laplace transform of Eq. (1) is taken with respect to time, and the solution in transform space is found to be

$$\bar{u}(x, p) = u_0 z K_1(qz)[pK_1(q)]^{-1}, \tag{3}$$

where $z = e^{\beta x/2}$, $q = (4p/\beta^2 D_r)^{1/2}$, and K_1 is the modified Bessel function of the second kind of order one.

The inversion of Eq. (3) is obtained through the use of a contour integral in p space and noticing that $\bar{u}(x, p)$ has a branch point at the origin.[9] The result of the inversion is

$$u(x, t) = u_0 \left(1 - \frac{2z}{\pi} \int_0^\infty I(z, \tau, k)\, dk\right), \tag{4}$$

where

$$I(z, \tau, k) \equiv \frac{e^{-k^2\tau}}{k} \left(\frac{N_1(kz)J_1(k) - J_1(kz)N_1(k)}{J_1^2(k) + N_1^2(k)}\right); \tag{5}$$

J_1 and N_1 are Bessel and Neumann functions, respectively, of order one, k is a dummy variable of integration, and τ is the dimensionless time variable, $\tau = \frac{1}{4}\beta^2 D_r t$. The integral can not be evaluated analytically, except in the special case $t = 0$, where, of course, the required initial condition (2) is recovered.

A short time approximation can be evaluated by using the asymptotic expansion for K_1 in Eq. (3)

as $p \to \infty$, since p and t are inversely related.[9,10] The result of inverting the expansion for Eq. (3) is found to be [9,10]

$$u(x,t) \simeq u_0 z^{1/2} \{ \mathrm{erfc}[(z-1)/2\tau^{1/2}] - 3\tau^{1/2}(z-1) i\,\mathrm{erfc}[(z-1)/2\tau^{1/2}]/4z + \tau(33z^2 - 18z - 15) i^2 \times \mathrm{erfc}[(z-1)/2\tau^{1/2}]/32z^2 \}, \quad (6)$$

which is valid for $\tau \ll 1$. The repeated integrals of the complementary error function

$$i\,\mathrm{erfc}(y) = \int_y^\infty \mathrm{erfc}(q)\,dq,$$

$$i^2\,\mathrm{erfc}(y) = \int_y^\infty i\,\mathrm{erfc}(q)\,dq,$$

are tabulated.[9,10] Equation (6) has similarities to the solution of the diffusion equation for a constant thermal-diffusion coefficient D, with the same initial and boundary conditions, namely,

$$u_T(x,t) = u_0\,\mathrm{erfc}[x/2(Dt)^{1/2}]. \quad (7)$$

With $D = D_r$, for small x Eqs. (6) and (7) predict $u(x,t) > u_T(x,t)$, while for large x, $u(x,t)$ falls to zero much more rapidly than $u_T(x,t)$.

Equation (4) can be evaluated numerically using a simple trapezoidal rule to calculate the infinite integral, due to the rapid decay of the integrand. We have made this calculation for various values of τ, as shown by the solid lines in Fig. 1. Also plotted (dashed line) is the thermal solution for $D = D_r$ and the value of time, $t = 4(\beta^2 D_r)^{-1}$. It is seen again that $u(x,t)$ is greater than $u_T(x,t)$ for the region $x < 1/\beta$, but for $x \gg 1/\beta$, $u(x,t) \ll u_T(x,t)$. It is clear that for any choice of parameters to characterize a thermal-diffusion profile, in comparison to the enhanced-diffusion profile, thermal diffusion results in a more slowly changing profile. The sharper profile displayed for irradiation-enhanced diffusion is characteristic of the fall-off of the diffusion coefficient (and increase in the average jump time) with distance inside the sample which causes the impurity atoms to tend to penetrate primarily near the surface.

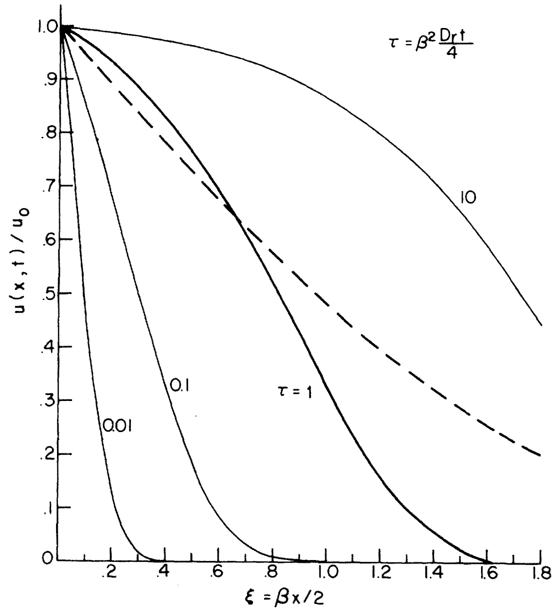

FIG. 1. Normalized concentration $u(x,t)/u_0$ vs normalized depth ξ into the sample. The solid lines give the results for the enhanced diffusion coefficient, $D(x) = D_r e^{-\beta x}$, from Eqs. (4 and 5) for various effective times τ. The dashed line gives the results for a normal, thermally activated diffusion coefficient, $D(x) = D_r$, for $\tau = 1$.

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[1] A great number of the early experimental references are contained in recent reviews (Refs. 2–4) and will not be repeated here.

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