Impurity diffusion in a semi-infinite region

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We describe the problem of impurity diffusion in a semi-infinite region in the context of a model that caricatures the Fokker-Planck equation. The solution obtained for the surface flux is an improvement over that found using the diffusion equation in two important respects: The short-time behavior is better and additional information is found regarding the physical process at the substrate-reactant interface.

I. DIFFUSION EQUATION THEORY

We have recently made use of a simple model to investigate several problems usually described by the solution of the diffusion equation (DE) for a specified boundary condition.[1,2] This previous work has focused on situations involving an absorbing boundary for which the correct boundary condition, that no particles emerge from the boundary, cannot be prescribed since the DE description includes only position and time but not velocity. In the present Brief Report we consider a different type of boundary value problem, where the DE description does properly treat the boundary condition, for which the model still provides an improved description. The model allows us a more believable description at short times, for which it is known the DE is qualitatively incorrect,[3] and also allows us a more complete understanding of the physical processes taking place.

The specific problem we consider is impurity diffusion in a semi-infinite region.[4] A dopant is initially uniformly distributed in a substrate which at $t=0$ is allowed to react with a gas under controlled conditions that insure a local equilibrium will be maintained at the substrate-gas interface where the dopant concentration is $c_0 < c_\infty$, with c_∞ the initial concentration. This can be treated as a one-dimensional problem and the DE solution for the surface flux is

$$j_{\mathrm{DE}} = -(c_\infty - c_0)(D/\pi t)^{1/2} , \tag{1}$$

with D the diffusion coefficient for the dopant in the substrate. This result is clearly problematic at very short times; also, the DE does not allow us to determine the separate contributions to the flux of dopant exiting and reentering the substrate.

II. MODEL EQUATION DESCRIPTION

A description which allows a more accurate description of short times and permits us to distinguish between flux components is provided by the Fokker-Planck equation[3] (FPE) which includes velocity as well as position and time. The difficulty in obtaining solutions for this equation in specific situations has motivated us to consider a simple caricature of this equation[1] that includes its most pertinent feature relative to our present concern—information about particle velocities. We have also shown[5] that the model is equivalent to the lowest level of approximation in a systematic representation of the exact FPE solution in the same way that Bhatnagar, Gross, and Krook (BGK) model solutions are equivalent to approximations of exact solutions to the linearized Boltzmann equation.[6]

We consider the diffusing particle to move with velocities $\pm s$ with distribution functions $u_+(x,t)$ and $u_-(x,t)$ so that the diffusant density is $w(x,t) = u_+(x,t) + u_-(x,t)$ and the flux is now an independent quantity given by $sv(x,t)$ with $v(x,t) = u_+(x,t) - u_-(x,t)$. The kinetic description is given by

$$\frac{\partial u_\pm}{\partial t} \pm \frac{s\,\partial u_\pm}{\partial x} = \beta(u_\mp - u_\pm) , \tag{2}$$

where β is related to the friction coefficient and $D = s^2/2\beta$. This equation is to be solved here subject to the boundary condition $w(x,0) = c_\infty$, $w(0,t) = c_0 < c_\infty$. In particular, we want to find the surface flux $j(0,t) = sv(0,t)$; this quantity follows directly from the results given in the Appendix of Ref. 1,

$$\begin{aligned} j(0,t) = sv(0,t) &= s(c_0 - c_\infty)\left\{1 - \beta\int_0^t d\tau\, e^{-\beta\tau}[I_0(\beta\tau) - I_1(\beta\tau)]\right\} \\ &= s(c_0 - c_\infty)\exp(-\beta t) I_0(\beta t) , \end{aligned} \tag{3}$$

where I_n is the modified Bessel function of order n. At long times the preceding result reduces to the DE result Eq. (1) but for $\beta t \ll 1$ this result behaves quite differently.

III. DISCUSSION

In addition to providing an acceptable description of the initial surface flux development the model also allows us to determine the separate contributions to this quantity from exiting and reentering dopant particles. The former is just $su_-(0,t)$ while the latter is $su_+(0,t)$. From (3) and the boundary condition $u_+(0,t) + u_-(0,t) = c_0$ we easily find

$$su_-(0,t) = \tfrac{1}{2} c_\infty e^{-\beta t} I_0(\beta t) , \tag{4}$$

$$su_+(0,t) = \tfrac{1}{2}(2c_0 - c_\infty) e^{-\beta t} I_0(\beta t) . \tag{5}$$

This problem clearly illustrates that even in situations where the DE provides a physically correct description of the boundary condition that the model description is more accurate (in time-dependent problems) and richer in detail. Additional results, including the dopant concentration in the substrate interior, also follow directly from the results of Ref. 1.

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