

Ionization enhanced diffusion*

D. Peak

Physics Department, Union College, Schenectady, New York 12308

J. W. Corbett†

Physics Department, State University of New York at Albany, Albany, New York 12222

J. C. Bourgoin

Laboratoire de Physique, Ecole Normale Supérieure, University of Paris VII, 75221 Paris, France

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The general three-dimensional diffusion equations, along with the corresponding tensor diffusivities, are established for the normal ionization-enhanced diffusion mechanism (which is equivalent to a general two-channel diffusion mechanism) and for the Bourgoin mechanism, the latter being explicitly developed for the diamond lattice.

I. INTRODUCTION

There have been a number of papers¹⁻²⁰ dealing with various aspects of enhanced diffusion mechanisms in semiconductors. In an earlier paper¹¹ we established the *one-dimensional* diffusion equations and diffusion coefficient parametrization for the normal ionization-enhanced diffusion mechanism^{10,20} and for the Bourgoin mechanism.^{8-10,20} That treatment was in terms of a classical description of the diffusing species. In this paper, by expressing the macroscopic transition rates in terms of the quantum states of the defect-lattice system, we relate the macroscopic diffusion equations to the microscopic processes giving rise to these enhancement mechanisms. The diffusivities so obtained are expressed in full tensor form, as is appropriate for lattice diffusion. In particular, we derive the explicit form of the Bourgoin enhanced diffusivity for the important case of defect migration on the diamond lattice.

II. MICRO- AND MACROSTATES OF A DEFECT-LATTICE SYSTEM

We begin by reviewing the essential features of the quantum mechanical description of the migration of a point defect through a solid lattice. In particular, we consider an infinite crystal containing a single point defect.²¹ Let H , the Hamiltonian of the system, be written as

$$H = H_L + H_0(n) + H_I(n), \quad (1)$$

where H_L is the perfect crystal Hamiltonian, $H_0(n)$ is the Hamiltonian of a point defect which is localized at site n and which can move independently of the rest of the lattice, and $H_I(n)$ represents the defect-lattice interaction due to the defect at n . We construct states $|ni\rangle$ such that

$$[H_L + H_0(n)]|ni\rangle = \epsilon_{ni}|ni\rangle; \quad (2)$$

each $|ni\rangle$ can be expressed as a product state involving the phonon states of the perfect crystal and the localized eigenstates of $H_0(n)$. The $|ni\rangle$ can then be utilized as a complete set of orthogonal states in order to expand a general state of the defect-lattice system, $|\Psi\rangle$, as

$$|\Psi(t)\rangle = \sum_{n,i} a_{ni}(t) \exp(-i\epsilon_{ni}t/\hbar) |ni\rangle. \quad (3)$$

Now, the time development of $|\Psi\rangle$ is determined by

$$H|\Psi\rangle = i\hbar \partial_t |\Psi\rangle; \quad (4)$$

the effect of $H_I(n)$ is to mix $|ni\rangle$ states with states $|mj\rangle$ corresponding to defect states localized at different lattice sites. Since the probability density that the system is in state $|ni\rangle$ at time t is

$$|\langle ni|\Psi(t)\rangle|^2 = |a_{ni}(t)|^2, \quad (5)$$

then if $|\Psi(0)\rangle$ is specified to be $|ni\rangle$, $|a_{mj}(t)|^2$ is the probability density that the system will have undergone a transition from the initial state $|ni\rangle$ to the final (i. e., at time t) state $|mj\rangle$. Furthermore, the transition rate in this case, W_{ni}^{mj} , is

$$W_{ni}^{mj} = \lim_{t \rightarrow 0} |a_{mj}(t)|^2 / t. \quad (6)$$

It is easy to show that

$$i\hbar \dot{a}_{mj} = \epsilon_{mj} a_{mj} + \sum_{n,i} a_{ni} \exp[-i(\epsilon_{ni} - \epsilon_{mj})t/\hbar] \times \langle mj|H_I(n)|ni\rangle, \quad (7)$$

which can be solved to first order in $H_{I(n)}$, for example, to yield the well-known result²²

$$W_{ni}^{mj} \approx 2\pi |\langle mj|H_I(n)|ni\rangle|^2 \delta(\epsilon_{ni} - \epsilon_{mj})/\hbar. \quad (8)$$

In what follows, we will be interested in the *macroscopic* defect concentration localized at n at time t , $c_n(t)$, and the *macroscopic* transition rate w_{mn} . When the defect concentration is sufficiently dilute, these quantities are defined in terms of appropriate thermal averages of the microscopic quantities discussed above by

$$c_n(t) \equiv \sum_i P_i |a_{ni}(t)|^2 \quad (9)$$

and

$$w_{mn} \equiv \sum_{i,j} P_i W_{mi}^{nj}; \quad (10)$$

here P_i is the probability of state i occurring in a statistical ensemble appropriate to the thermodynamic

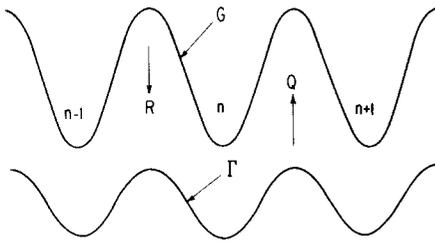


FIG. 1. The defect potential about site n in a one dimensional lattice for two different defect charge states (G and Γ), in the normal ionization enhanced (or simple two channel) diffusion model. R represents the total G to Γ transition rate, Q the total Γ to G rate.

conditions.

We proceed to analyze the time rates of change of defect concentrations, defined as in (9), in the subsequent sections.

III. ORDINARY DIFFUSION

In ordinary diffusion, the macroscopic concentration at site n changes in time owing to the difference between transitions into n and those out of n . Thus we write

$$\partial_t c_n = \sum_m (w_{mn} c_m - w_{nm} c_n). \tag{11}$$

We assume that the defect-lattice interaction is symmetrical; that is, we suppose

$$W_{ni}^{mj} = W_{mi}^{nj}. \tag{12}$$

Then (11) becomes just

$$\partial_t c_n = \sum_m w_{mn} (c_m - c_n). \tag{13}$$

Because of the mixing of defect states at different sites due to the interaction between defect and lattice, the defect states can be said to propagate through the lattice with wave vectors \mathbf{k} . If we denote the position of the n th lattice site by \mathbf{r}_n , and write $\mathbf{r}_m = \mathbf{r}_n + \mathbf{l}_m$, where \mathbf{l}_m is the position of the m th site with respect to the n th site, then whenever $\mathbf{k} \cdot \mathbf{l}_n \ll 1$ the lattice structure is irrelevant and the above difference Eq. (13) can be replaced by a differential equation in the spatial variables. In the so-called continuum ("short jump") limit

$$c(\mathbf{r}_m) = c(\mathbf{r}_n) + \mathbf{l}_m \cdot \nabla c(\mathbf{r}_n) + \frac{1}{2} \nabla \cdot \mathbf{l}_m \mathbf{l}_m \cdot \nabla c(\mathbf{r}_n) + \dots, \tag{14}$$

and (13) is equivalent to

$$\partial_t c \approx \nabla \cdot \bar{D} \cdot \nabla c, \tag{15}$$

where

$$\bar{D} = \frac{1}{2} \sum_m w_{mn} \mathbf{l}_m \mathbf{l}_m. \tag{16}$$

(The first order terms in the sum vanish because each term $\mathbf{l}_m w_{mn}$ is cancelled by an identical term $-\mathbf{l}_m w_{mn}$.)

In one dimension, where $\mathbf{l}_m = (m - n)a$ and a is a lattice constant, (15) and (16) reduce to

$$\partial_t c(x, t) = D \partial_x^2 c(x, t) \tag{17}$$

and

$$D = \frac{1}{2} \sum_m w_{mn} (m - n)^2 a^2, \tag{18}$$

respectively.

IV. TWO CHANNEL DIFFUSION

One means of enhanced diffusion involves two channels for thermally activated diffusion. In our discussion the two channels are two different charge states of the same defect, but a similar analysis may be made for dissociative diffusion²³⁻²⁵ (where one channel is an interstitial channel and the other a substitutional channel) or similar systems. We note that the defect-lattice interaction can result in a change in charge state of the defect and suppose in this section that in this change the minimum of the potential the defect moves in is not shifted (see Fig. 1). We also assume that the sets of the states contributing to each charge state are disjoint and identifiable. Then we may meaningfully write

$$c_n = \sum_i P_i |a_{ni}(t)|^2,$$

for the G state, and

$$\gamma_n = \sum_\mu P_\mu |a_{n\mu}(t)|^2,$$

for the Γ state. Let us suppose that the charge state change matrix elements $\langle ni | H_I | m\mu \rangle$ are dominated by the single site terms $\langle ni | H_I | n\mu \rangle$, and that these are n independent. Then

$$\partial_t c_n = \sum_m w_{mn} (c_m - c_n) - R c_n + Q \gamma_n \tag{19}$$

and

$$\partial_t \gamma_n = \sum_m \psi_{mn} (\gamma_m - \gamma_n) + R c_n - Q \gamma_n, \tag{20}$$

where

$$w_{mn} = \sum_{i,j} P_i W_{mi}^{nj},$$

$$\psi_{mn} = \sum_{\mu,\nu} P_\mu W_{m\mu}^{n\nu},$$

$$R = \sum_{\mu,i} P_i W_{ni}^{n\mu},$$

and

$$Q = \sum_{\mu,i} P_\mu W_{ni}^{n\mu}.$$

Now, if charge exchange occurs much more frequently than other processes, local reaction equilibrium between G states and Γ states will be approximately observed. As a result, the transport of defect from site to site can be monitored by observing only one of the charge states, since the G and Γ defects will essentially diffuse as one. Thus, we can define new concentrations \bar{c}_n and $\bar{\gamma}_n$ which satisfy

$$R \bar{c}_n = Q \bar{\gamma}_n \tag{21}$$

and the summed kinetic equation

$$\partial_t(\bar{c}_n + \bar{\gamma}_n) = \sum_m [w_{mn}(\bar{c}_m - \bar{c}_n) + \psi_{mn}(\bar{\gamma}_m - \bar{\gamma}_n)]. \quad (22)$$

These new concentrations can be expected to be appreciably different from c_n and γ_n only throughout small regions of the sample in question near its boundaries²⁶; the net defect transport rate through the lattice should be well approximated by that given by (21) and (22), i. e., by

$$(Q + R)\partial_t \bar{c}_n = \sum_m (Qw_{mn} + R\psi_{mn})(\bar{c}_m - \bar{c}_n). \quad (23)$$

In the continuum limit (23) becomes

$$\partial_t \bar{c} = \nabla \cdot \bar{D} \cdot \nabla \bar{c}, \quad (24)$$

where the effective, tensor diffusivity for the combined migration is

$$\begin{aligned} \bar{D} &= \frac{1}{2} \sum_m (Qw_{mn} + R\psi_{mn})(Q + R)^{-1} \mathbf{l}_m \mathbf{l}_m \\ &= (Q\bar{D}_G + R\bar{D}_\Gamma)(Q + R)^{-1}. \end{aligned} \quad (25)$$

In (25), \bar{D}_G and \bar{D}_Γ are the thermally activated diffusivities for the G - and Γ channels, respectively. In one dimension we have as before¹¹

$$D = (QD_G + RD_\Gamma)(Q + R)^{-1}, \quad (26)$$

where

$$D_G = \frac{1}{2} \sum_m w_{mn}(m - n)^2 a^2, \quad (27)$$

and so on. The macroscopic parametrization of D_G , D_Γ , R , and Q has been given elsewhere¹¹ and will not be repeated here.

V. BOURGOIN MECHANISM

A. General formalism

The essence of the Bourgoïn mechanism is that a change in the charge state of a defect is associated with a shift in the positions of the well minima to what were previously saddle point positions. In a given lattice each well site is surrounded by G saddle points, whereas each saddle point is surrounded by Γ wells.

If we sum (29) over all α , divide by Γ , and add the result to (28) we find that

$$\partial_t \bar{c}(\mathbf{r}_n) = \sum_m \left(\sum_{\alpha, \beta} \Gamma^{-2} \psi_{m\beta}^{n\alpha} [\gamma(\mathbf{r}_m + \mathbf{m}_\beta) - \gamma(\mathbf{r}_n + \mathbf{n}_\alpha)] + w_{mn} [c(\mathbf{r}_m) - c(\mathbf{r}_n)] \right) - Grc(\mathbf{r}_n) + \Gamma^{-1} r \sum_\alpha \sum_{n_\alpha} c(\mathbf{r}_{n_\alpha}). \quad (31)$$

Let us suppose that the continuum limit can be invoked. Then (31) becomes

$$\partial_t \bar{c} = \frac{1}{2} \sum_m \left(\sum_{\alpha, \beta} \Gamma^{-2} \psi_{m\beta}^{n\alpha} \nabla \cdot \lambda_{m\beta} \lambda_{m\beta} \cdot \nabla \gamma(\mathbf{r}_n + \mathbf{n}_\alpha) + w_{mn} \nabla \cdot \mathbf{l}_m \mathbf{l}_m \cdot \nabla c(\mathbf{r}_n) \right) + \frac{1}{2} \Gamma^{-1} r \sum_m' \nabla \cdot \mathbf{l}_m \mathbf{l}_m \cdot \nabla c(\mathbf{r}_n), \quad (32)$$

where $\lambda_{m\beta} = \mathbf{r}_m + \mathbf{m}_\beta - \mathbf{r}_n - \mathbf{n}_\alpha$, $\mathbf{l}_m = \mathbf{r}_m - \mathbf{r}_n$, and \sum' denotes a sum over only the nearest neighbor wells of \mathbf{r}_n .

As before, we assume that charge exchange occurs at a much higher rate than thermal diffusion so that locally reaction equilibrium is approached. That is, we suppose that concentrations \bar{c} and $\bar{\gamma}$ which closely approximate c and γ , respectively, over the bulk of the sample, and which satisfy

We designate by \mathbf{r}_n the positions of the various wells and by $\mathbf{r}_n + \mathbf{n}_\alpha$, $\alpha = 1, 2, \dots, G$, the positions of the saddle points about \mathbf{r}_n ; note that the sets $\{\mathbf{n}_\alpha\}$ may be different for different n -values and that there are Γ equivalent labels for each saddle point position. Now the concentration of G -state defect localized at \mathbf{r}_n changes in time according to the relation

$$\begin{aligned} \partial_t c(\mathbf{r}_n) &= \sum_m w_{mn} [c(\mathbf{r}_m) - c(\mathbf{r}_n)] \\ &\quad - Grc(\mathbf{r}_n) + q \sum_\alpha (\mathbf{r}_n + \mathbf{n}_\alpha), \end{aligned} \quad (28)$$

while the Γ -state concentration associated with site $\mathbf{r}_n + \mathbf{n}_\alpha$ changes according to

$$\begin{aligned} \partial_t \gamma(\mathbf{r}_n + \mathbf{n}_\alpha) &= \sum_m \sum_\beta \Gamma^{-1} \psi_{m\beta}^{n\alpha} [\gamma(\mathbf{r}_m + \mathbf{m}_\beta) - \gamma(\mathbf{r}_n + \mathbf{n}_\alpha)] \\ &\quad - \Gamma q \gamma(\mathbf{r}_n + \mathbf{n}_\alpha) + r \sum_{n_\alpha} c(\mathbf{r}_{n_\alpha}). \end{aligned} \quad (29)$$

In (28) and (29) we have employed the following notation: w_{mn} is defined in the same manner as in the preceding section; $\psi_{m\beta}^{n\alpha}$ is analogous to the ψ_{mn} of the preceding section, but now involves matrix elements of the form $\langle \mathbf{r}_m + \mathbf{m}_\beta; \mu | H_I | \mathbf{r}_n + \mathbf{n}_\alpha; \nu \rangle$; r and q are similar to the R and Q used previously, except now these rates refer to only part of the total charge exchange rate localized at \mathbf{r}_n —that is, r and q involve matrix elements of the form $\langle \mathbf{r}_n; i | H_I | \mathbf{r}_n + \mathbf{n}_\alpha; \mu \rangle$ (we assume that these matrix elements are n - and α independent); the Γ^{-1} in (29) is necessary to compensate for the Γ -fold counting of each saddle point inherent in the double sum over m and β ; and, lastly, the final sum in (29) is over the Γ wells immediately surrounding $\mathbf{r}_n + \mathbf{n}_\alpha$.

We proceed in analogy with the discussion of the simple two channel mechanism given above. We can define an average total defect concentration at \mathbf{r}_n by assuming that the Γ -state concentration at any point is shared equally by Γ surrounding sites \mathbf{r}_n . Then the average total defect concentration at \mathbf{r}_n is

$$\bar{c}(\mathbf{r}_n) \equiv c(\mathbf{r}_n) + \Gamma^{-1} \sum_\alpha \gamma(\mathbf{r}_n + \mathbf{n}_\alpha). \quad (30)$$

$$Gr\bar{c}(\mathbf{r}_n) = q \sum_\alpha \bar{\gamma}(\mathbf{r}_n + \mathbf{n}_\alpha), \quad (33)$$

can be defined. Then the total defect migration can be traced by studying just one channel. For example, in the G channel (32) reduces to an expression in \bar{c} , identical in form to that of (24), but where now the tensor

diffusivity \bar{D} is

$$\bar{D} = (Q\bar{D}_G + R\bar{D}_\Gamma)(Q + R)^{-1} + \bar{D}_B; \quad (34)$$

here $Q = \Gamma q$ is the total Γ to G rate, $R = Gr$ is the total G to Γ rate,

$$\bar{D}_G = \frac{1}{2} \sum_m w_{mn} \mathbf{l}_m \mathbf{l}_m,$$

$$\bar{D}_\Gamma = \frac{1}{2} \sum_m \sum_\beta \Gamma^{-1} \psi_{m\beta}^{\alpha} \lambda_{m\beta} \lambda_{m\beta},$$

and \bar{D}_B is the Bourgoïn diffusivity,

$$\bar{D}_B = \left(\frac{1}{2} \sum_m \mathbf{l}_m \mathbf{l}_m \right) (QR)(Q + R)^{-1} (G\Gamma)^{-1}. \quad (35)$$

The one dimensional case is depicted in Fig. 2. G states are localized at integral multiples of a , Γ states half-way between. In one dimension, \bar{D}_Γ becomes just

$$D_\Gamma = \frac{1}{2} \sum_m \psi_{mn} (m - n)^2 a^2,$$

where the matrix elements contributing to ψ_{mn} are $\langle m + \frac{1}{2}; \mu | H_I | n + \frac{1}{2}; \nu \rangle$; \bar{D}_G becomes the same as in (27). The Bourgoïn diffusivity in one dimension, with $G = \Gamma = 2$, is

$$D_B = QR(Q + R)^{-1} (a^2/4), \quad (36)$$

a result which has been noted previously.¹¹

B. The diamond lattice

There are two networks in the diamond lattice on which it has been suggested^{9-11,15} that the Bourgoïn mechanism may operate. The first is the network consisting of the tetrahedral and hexagonal interstitial sites; the second is the network of substitutional sites and the sites half-way between these substitutional sites—the so-called bond-centered sites. As can be readily verified by considering the diamond lattice, the topologies of both networks are the same, each network being just shifted with respect to the other. We illustrate the various jump vectors in Fig. 3. The $\{\mathbf{l}_G\}$ generate the set of substitutional sites which are nearest to a given substitutional site. Specifically, the \mathbf{l}_G will be of the form $\mathbf{l}_G = \sqrt{a} [1, 1, 1]/4$, for example, where the bracketed numerals are the components of the vector along the cubic axes of the crystal. The $\{\lambda_\Gamma\}$ generate the set of $G + \Gamma = 6$ bond-centered sites which are nearest to a given bond-centered site, e.g., $\lambda_\Gamma = \sqrt{a} [1, 1, 0]/4$, etc.

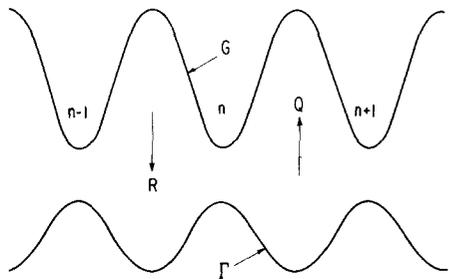


FIG. 2. The defect potential about site n in a one dimensional lattice for two different charge states, in the Bourgoïn enhanced diffusion model.

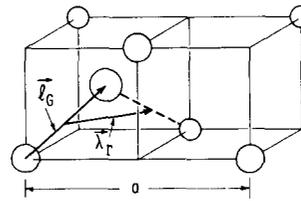


FIG. 3. A portion of the diamond lattice displaying typical displacement vectors between nearest-neighbor split interstitial sites (\mathbf{l}_G) and nearest-neighbor bond-centered sites (λ_Γ).

From the equations in the preceding section, using these vectors and assuming we need consider only nearest neighbor jumps, we obtain

$$\nabla \cdot \bar{D}_i \cdot \nabla = D_i \nabla^2, \quad i = G, \Gamma, B, \quad (37)$$

where

$$D_G = 3a^2 w/8, \quad (38)$$

$$D_\Gamma = 3a^2 \psi/8, \quad (39)$$

and

$$D_B = 3a^2 QR [32(Q + R)]^{-1}; \quad (40)$$

w and ψ are the probabilities of thermally activated nearest neighbor jumps in the respective channels. Note that diffusion in the diamond lattice is isotropic, as might be expected. Thus, in summary, we can write

$$\partial_t \bar{c} = [(QD_G + RD_\Gamma)(Q + R)^{-1} + D_B] \nabla^2 \bar{c}$$

for the G -state diffusion equation for the Bourgoïn mechanism in the diamond lattice.

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