

## The Effect of Dislocation Pipe Diffusion on Electro-Migration-Induced Breakdown in an FCC Structure

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(Received June 21, 1991)

### 면심입방구조에서 Electro-Migration-Induced Breakdown에 대한 전위파이프 확산의 영향

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(1991년 6월 21일 접수)

#### ABSTRACT

The mobility and diffusivity in an edge dislocation in an FCC crystal formed by the removal of one half of a (100) plane were evaluated in an applied field by analyzing a vacancy tight binding model using Stark's matrix technique. A model of an edge dislocation in an FCC crystal was constructed for a [100] Burgers vector where vacancy transport along the edge of the extra half plane of ions was considered. The model considered a tight binding approximation of the vacancy to the compressed region of the core and carried the calculation to the limit of an infinite length of dislocation. The diffusivity and the ratio of mobility to diffusivity were found to increase without bounds in the limit where the correlation factor becomes zero. In contrast, as the correlation factor became unity, the diffusivity became zero and the ratio of mobility to diffusivity became unity associated with the uncorrelated limit of  $1/kT$ . This implied that the phenomenon was not unique to the crystal structure but was unique to edge dislocations with vacancy tight binding.

#### 요 약

(100)면의 반이 없어 생긴 면심입방결정 칼날전위의 가동성과 확산계수를 전자장이 있는 조건에서 공공결속 모델과 Stark의 계산방법을 이용 이론적으로 분석되었다. 면심입방결정 칼날전위의 모델은 공공이 이온의 잉여 반면을 따라 이동하는 [100] 버거스 벡터를 중심으로 만들어졌다. 공공결속모델은 공공과 전위핵의 수축된 부분의 결속을 전위의 모한대까지 고려되었다. 상관계수가 0일 때 가동성과 확산계수의 비와 가동성은 무한대로 증가하였다. 반대로 상관계수가 1일 때는 확산계수는 0이 되었고,  $kT$  곱하기 가동성과 확산계수의 비는 1이 되었다. 위 사실은 결정구조에는 관련이 없지만 칼날전위에는 꼭 일어나는 독특한 현상이었다.

#### 1. Introduction

Solid state diffusion of atoms has been studied extensively through evaluation of several different crystal defect mechanisms. Generally, diffusion of species within a system was characterized by the diffusion coefficient. The technique used to analytically determine the diffusion coefficient was to mathematically follow the random motion of a tracer atom through the crystal

matrix. However, it has been found that this motion may not indeed be totally random. Therefore, a correlation factor became necessary to describe actual diffusion. The correlation effect allowed for an atom to jump randomly. However, because of the influence of defects or impurities, sequential jumps were more likely to be in opposite directions thus having a smaller overall net displacement. The correlation factor, as defined by Bardeen and Herring<sup>1)</sup>, was the ratio of the

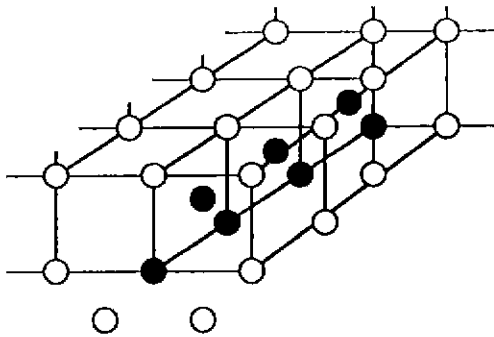


Fig. 1. Atomic model of edge dislocation on FCC structure.

diffusion coefficient for mass transport of a species to the self diffusion coefficient calculated on the basis of totally random motion.

An analytical method of evaluation the diffusivity and correlation factor was developed by Bardeen and Herring<sup>1</sup> based on a thermodynamic and kinetic approach to the Kirkendall effect. This method was expanded by Howard<sup>2</sup> using matrices of probabilities based on several different possible jump vectors or "types" of jumps. Stark<sup>3</sup> further expanded the random walk matrix method developed by Howard<sup>2</sup> and applied it to the case of a dilute solute tracer in an FCC lattice which diffuses by a vacancy mechanism. Calculation of the average jump frequency was combined with the correlation factor calculation to directly determine the diffusivity.

Robinson and Peterson<sup>4,5</sup> developed an analytical solution for the correlation factor in the case of FCC lattice dislocation pipe diffusion with a vacancy mechanism. This analysis was achieved by defining the crystallographic model and using Howard's general matrix method. Stark<sup>6</sup> made a more rigorous evaluation to eliminate these limitations by redefining the site classes and expanding the matrices. Stark<sup>7</sup>, therefore, applied this technique to dislocation pipe diffusion in a simple cubic structure by a vacancy mechanism. Two extreme approximations were approached. First, tight binding of the vacancy to the dislocation pipe core. Second, loose binding of the vacancy to the dislocation pipe core. The loose binding analysis was analogous to the case studied by Robinson and Peterson<sup>4,5</sup> and Stark<sup>6</sup> for FCC dislocation pipe self diffusion.

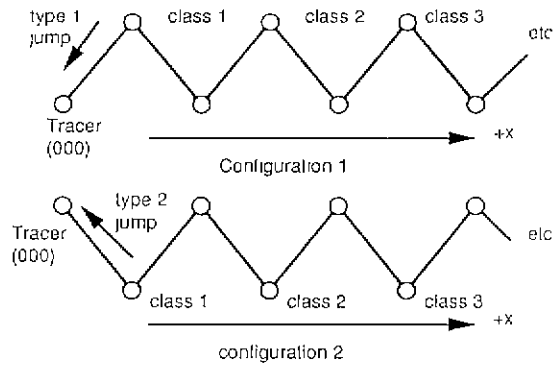


Fig. 2. Simplified 1-dimensional diffusion model.

Stark<sup>8</sup> also evaluated the diffusivity and mobility for dislocation pipe diffusion in a simple cubic lattice structure using the method described in Ref.<sup>3</sup> for diffusivity and the technique developed by Stark and Manning<sup>9</sup> for the mobility. The results indicated that as the tight binding limit was approached for an infinitely long dislocation pipe, the correlation factor approached zero. However, the diffusivity and the ratio of mobility to diffusivity both became very large. The mobility to diffusivity ratio was found to be proportional to the reciprocal of the correlation factor for all jump frequency responses causing the unusual behavior. This implied that the vacancy wind became infinite in this limit. Thus, for a specific material at certain conditions in an applied field that exhibited vacancy tight binding to dislocation cores, it would be expected to observe very rapid diffusion. As the correlation factor became unity, the diffusivity became zero because there were no available vacancies. However, the ratio of mobility to diffusivity became unity associated with the uncorrelated limit of  $1/kT$  since for every vacancy that did indeed move the tracer. It will do so with only one tracer jump. It is the intention of this study to extend the calculation of the correlation factor in an FCC crystal to yield an expression for the diffusivity and the mobility in an applied field.

## 2. Model

The correlation factor was analyzed using some modifications on the model outlined by Robinson and Peterson<sup>4,5</sup>. The edge dislocation was defined by a Bur-

**Table 1.** Definition of the Jump Frequencies

Initial location	Final location	Frequency
in the dislocation pipe	in the dislocation pipe	$\omega_2$
in the dislocation pipe	out of the dislocation pipe	$\omega_3$
out of the dislocation pipe	in the dislocation pipe	$\omega_4$

gers vector of  $b=a[100]$ . Specifically, the dislocation was formed by the removal of one half of a (100) plane. Considering the stress gradient around the dislocation pipe caused by its existence, it was expected that vacancies will be attracted to the compressed area in and surrounding the pipe. Also, Robinson and Peterson stated that the vacancy-dislocation binding energy decreased by an order of magnitude within two nearest neighbor distances from the dislocation core. Therefore, the model encompasses the dislocation pipe, and all nearest neighbor sites to these, as shown in Fig. 1.

In the tight binding analysis, where the vacancy was essentially trapped in the lattice sites of the bottom edge of the extra half plane of atoms, the model was simplified. There are two possible configurations of tracer-vacancy dislocation pipe that can lead to a vacancy tracer exchange. These are two possible configurations of tracer-vacancy dislocation pipe that can lead to a vacancy tracer exchange. These are shown in Fig. 2. In configuration 1, the tracer occupies a lattice site with 10 nearest neighbors and vacancy one with 12 nearest neighbors. Configuration 2 is the opposite. All sites shown are on the bottom edge of the extra half plane directly above the dislocation pipe. The diffusion direction shown by the positive  $x$  axis is along the  $\langle 100 \rangle$  direction of the lattice. It is assumed that only nearest neighbor exchanges between vacancy and atom are possible.

The vacancy positions and the associated jump frequencies are listed in Table 1. In this way,  $\omega_2$  describes the jump frequency along the dislocation pipe,  $\omega_3$  the vacancy escape frequency, and  $\omega_4$  the vacancy arrival frequency.

The probability of a type 1 jump, where the vacancy goes from a 12 nearest neighbor site to a 10 nearest neighbor site is,

$$y = \frac{\omega_2}{2\omega_2 + 10\omega_3} \quad (1)$$

and the opposite jump from 10 nearest neighbors to 12 nearest neighbors is,

$$y = \frac{\omega_2}{2\omega_2 + 8\omega_3} \quad (2)$$

It is necessary to consider the influence of the field upon the matrices  $A$ ,  $B$  and their manipulations to calculate the mobility and diffusivity. To that effect, consider the effect of the field strength (parallel to the dislocation core) upon the jump probability for a single vacancy jump. Thus,

$$z^+ = \frac{\omega_T^+}{\omega_T^+ + \omega_2^- + 2\omega_3^+ + 2\omega_3^- + 4\omega_3^0} \quad (3)$$

$$y^+ = \frac{\omega_T^+}{\omega_T^+ + \omega_2^- + 3\omega_3^+ + 3\omega_3^- + 4\omega_3^0} \quad (4)$$

where the superscripts  $+$  or  $-$  indicate the direction of the atom motion in relation to the force and  $0$  indicates motion normal to the force and subscript  $T$  indicates tracer-vacancy exchange.

### 3. Calculations

In this approximation to the motion of the vacancy around a tracer ion at the origin, there is no possibility of a sequence of two tracer jumps in the same direction, the so-called parallel jump. The effective distance ( $S$ ) that a tracer can migrate in an applied field divided by the lattice parameter from a single vacancy and the vacancy arrival rate ( $v$ ) that the vacancy arrives at the tracer by migration from a source having never been there before contain nonlinear terms resulting from the product of probability terms. In the expansion of the field effect it is therefore important to delete all nonlinear terms in the force. If one expands the terms to exclude nonlinear field effects, then to the first order in the applied field one finds  $dv$  and  $dS$  are proportional to the force to the first power. The

mobility of tracer was expressed using the expression of the tracer velocity<sup>31</sup>,

$$\mu = \frac{b}{E[v_d S + S_d v]} \quad (5)$$

**3.1. Correlation factor**

In the case of any type of cubic crystal, the correlation factor is isotropic so that it is only necessary to calculate it with respect to any one of the principle axes. Howard's formulation<sup>29</sup> for correlation factor was modified using the tight binding model and Stark's matrix<sup>31</sup>. The correlation factor is a dot product of the partial correlation factors and the ratio of the number of jumps of each type to the total number of jumps. The partial correlation factors,  $f_1$  and  $f_2$ , are calculated by,

$$F = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = (1-P)(+P)^{-1} l \quad (6)$$

where P is an N×N matrix with elements  $P_{ij}$  equal to the universal probability of a jump of type i being followed by a jump of type j. l is a unit column matrix. And the ratio of the number of jumps of each type to the the total number of jumps was given by Stark<sup>31</sup>. Therefore, the general expression of f is,

$$f = \frac{l^T v P(1+P)^{-1} l}{l^T n P(1-P)^{-1} l} \quad (7)$$

where the vacancy arrival rate,  $v_j$ , is expressed by,

$$v_1 = H_2 (1-B_3)^{-1} T_2 \quad \text{and} \quad v_2 = H_1 (1-A_3)^{-1} T_1 \quad (8)$$

where  $H_j$  is a row vector of occupation probabilities for sites in configuration j and  $T_j$  is a column vector of the number of defect per unit time jumping from a set of other defects sites into a particular defect site and l is a N×N unit matrix. The matrices  $A_3$  and  $B_3$  have elements  $A_{3ij}$  and  $B_{3ij}$  which are the transition jump probabilities from the set of sites j into a particular site i. All tracer jumps are excluded. For this case,

$$H_1 = | 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ \dots | \quad \text{and} \quad H_2 = | 1 \ 0 \ 0 \ 0 \ 0 \ 0 \ \dots | \quad (9)$$

$$T_1 = 10V\omega_4 \begin{bmatrix} 1 \\ b \\ 1 \end{bmatrix} \quad \text{and} \quad T_2 = 10V\omega_4 \begin{bmatrix} b \\ 1 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} b \\ \vdots \\ 1 \end{bmatrix} \quad \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

$$A_3 = \begin{bmatrix} 0 & z & 0 & 0 & 0 & \dots \\ 0 & 0 & y & 0 & 0 & \dots \\ 0 & z & 0 & y & 0 & \dots \\ 0 & 0 & y & 0 & y & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{bmatrix} \quad \text{and} \quad B_3 = \begin{bmatrix} 0 & z & 0 & 0 & 0 & \dots \\ 0 & 0 & z & 0 & 0 & \dots \\ 0 & y & 0 & y & 0 & \dots \\ 0 & 0 & z & 0 & z & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{bmatrix} \quad (11)$$

Equation (8) was solved using Stark's method<sup>27</sup> for determining the inverse of an infinite matrix. The results are,

$$v_1 = 10V\omega_4 \frac{b+P_2}{1-P_1P_2} \quad \text{and} \quad v_2 = 10V\omega_4 \frac{1+bP_1}{1-P_1P_2} \quad (12)$$

In order to evaluate P, it is necessary to determine the matrices A and B. These were found by inspection and were in terms of atomic jump frequencies. These are,

$$A = \begin{bmatrix} 0 & z & 0 & 0 & 0 & \dots \\ y & 0 & y & 0 & 0 & \dots \\ 0 & z & 0 & y & 0 & \dots \\ 0 & 0 & y & 0 & y & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 0 & z & 0 & 0 & 0 & \dots \\ z & 0 & z & 0 & 0 & \dots \\ 0 & y & 0 & y & 0 & \dots \\ 0 & 0 & z & 0 & z & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{bmatrix} \quad (13)$$

The total jump sequence probabilities,  $P_1$  and  $P_2$ , were evaluated. And Stark's method<sup>27</sup> for taking the inverse of an infinite matrix was employed to describe the correlation factor. Therefore, the correlation factor was expressed as,

$$f = \frac{v_1 P_1 (1-P_2) + v_2 P_2 (1-P_1)}{v_1 P_1 (1+P_2) + v_2 P_2 (1+P_1)} \quad (14)$$

**3.2. Diffusivity**

To calculate diffusivity, Stark's matrix notation method<sup>31</sup> was used for this tight binding approximation. And this expression was combined with the correlation factor. The result is,

$$D = \frac{b^2 f f}{2} = \frac{b^2}{2} \left[ \frac{v_1 P_1 (1-P_2) + v_2 P_2 (1-P_1)}{(1-P_1 P_2)} \right] \quad (15)$$

**3.3. Mobility**

It is necessary to consider the influence of the field upon the matrices, A and B, and its manipulations to calculate the mobility and diffusivity. To that effect,

consider the effect of the field strength upon the jump probability for a single vacancy jump. Thus,

$$z^+ = z + dz \quad \text{and} \quad y^+ = y + dy \quad (16)$$

In order to evaluate  $P^+$ , it is necessary to consider the influence of the field upon the matrices A and B. These are,

$$A = \begin{vmatrix} 0 & z^- & 0 & 0 & 0 & \dots \\ y^- & 0 & y^- & 0 & 0 & \dots \\ 0 & z^+ & 0 & y^- & 0 & \dots \\ 0 & 0 & y^+ & 0 & y^- & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{vmatrix}$$

and  $B = \begin{vmatrix} 0 & z^- & 0 & 0 & 0 & \dots \\ z^+ & 0 & z^- & 0 & 0 & \dots \\ 0 & y^+ & 0 & y^- & 0 & \dots \\ 0 & 0 & z^+ & 0 & z^- & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{vmatrix} \quad (17)$

The total jump sequence probabilities are evaluated as,

$$P_1^+ = z^+(1-A)^{-1} \quad \text{and} \quad P_2^+ = y^+(1-B)^{-1} \quad (18)$$

By using Stark's matrix technique<sup>9)</sup> for taking the inverse of an infinite matrix, the total jump probabilities are,

$$P_1^+ = z^+ \alpha^{+-} \quad \text{and} \quad P_2^+ = y^- \alpha^{\sigma-} \quad (19)$$

$$\alpha^{+-} = \frac{(y^- z^+ - y^+ z^- + 1) - \sqrt{(y^+ z^- - y^- z^+ - 1)^2 - 4y^- z^-}}{2y^- z^-} \quad \text{and}$$

where

$$\alpha^{\sigma-} = \frac{(y^+ z^- - y^- z^+ + 1) - \sqrt{(y^- z^+ - y^+ z^- - 1)^2 - 4y^+ z^-}}{2y^+ z^-}$$

The vacancy arrival rate was found from the same matrix techniques as used in correlation factor. Therefore, the vacancy arrival rate was expressed by,

$$v_1 = 10V\omega_4 \frac{b + P_2}{1 - P_1^+ P_2^+} \quad \text{and} \quad v_2 = 10V\omega_4 \frac{1 + bP_1}{1 - P_1^- P_2^+} \quad (20)$$

The vacancy only approaches the tracer from one side so the results must be modified later to account for this deviation by introducing factors of 2 at appropriate places. The effective distance that a tracer can migrate in an applied field divided by the lattice parameter from a single vacancy is calculated depending on the tracer position, following the nomenclature of Stark

and Manning<sup>9)</sup>. The effective distances were found from,

$$S_1^+ = \frac{P_1^+(1-P_2^-)}{1-P_1^-P_2^-} \quad \text{and} \quad S_2^+ = \frac{P_2^+(1-P_1^-)}{1-P_1^-P_2^+} \quad (21)$$

Expansion of Equations (14), (15), (20), and (21) was used to show the effect of the field as follows:

$$z^+ = \frac{\omega_1^+}{(\omega_1^- + \omega_2^- + 2\omega_3^+ + 2\omega_3^- + 4\omega_3^0)} = \frac{\omega_2(1+e_2)}{(2\omega_2 + 8\omega_3)} = z + ez \quad (22)$$

$$y^+ = \frac{\omega_2^-}{(\omega_2^+ + \omega_2^- + 3\omega_3^+ + 3\omega_3^- + 4\omega_3^0)} = \frac{\omega_2(1+e_2)}{(2\omega_2 + 10\omega_3)} = y + ey \quad (22)$$

$$\alpha^{+-} = \frac{1 - \sqrt{1 - 4yz}}{2yz} + \frac{1 - \sqrt{1 - 4yz}}{2yz} \left[ \frac{dy}{y} - \frac{dz}{z} \right] = \alpha_0 + d\alpha \quad (24)$$

Similarly,

$$\alpha^{\sigma-} = \alpha_0 - d\alpha \quad (25)$$

$$P_1^+ = (z + ez)(\alpha + d\alpha) = P_1 + eP_1 \quad (26)$$

$$P_2^+ = (y + ey)(\alpha + d\alpha) = P_2 + eP_2 \quad (27)$$

$$v_1^+ = v_{10} + dv_1 \quad (28)$$

$$v_2^+ = v_{20} + dv_2 \quad (29)$$

$$S_1^+ = S_{10} + dS_1 \quad (30)$$

$$S_2^+ = S_{20} + dS_2 \quad (31)$$

$$e = \frac{Fb}{2kT} \quad (32)$$

where F is the force acting on the solvent atoms. F is equal to qE where q is the ionic charge in electromigration. The velocity of the tracer can be expressed as,

$V_i = \frac{b}{2} [(\text{Rate of defect arrives at tracer as perturbed by field}) \times (\text{probable distance the tracer moves}) + (\text{rate of defect arrives at tracer with no field}) \times (\text{field influence on probable distance the tracer moves})]$

$$= \frac{b}{2} [S_{10}dv_1 + S_{20}dv_2 + v_{20}dS_2 + v_{20}dS_2] \quad (33)$$

**Table 2.** Computer Calculation of Mobility and Diffusivity

g	P <sub>1</sub>	P <sub>2</sub>	f	D 10V <sub>0</sub> b <sup>2</sup>	$\frac{kT\mu}{Dq}$
0.0	1.0	1.0	0.0	∞	∞
0.0001	0.970	0.970	0.015	29.99	66.67
0.01	0.744	0.737	0.149	2.950	6.711
0.05	0.527	0.506	0.317	1.268	3.146
0.07	0.473	0.448	0.368	1.051	2.714
0.09	0.431	0.405	0.409	0.909	2.441
0.1	0.414	0.386	0.428	0.855	2.337
0.3	0.239	0.210	0.633	0.422	1.579
0.5	0.171	0.146	0.726	0.290	1.377
0.9	0.110	0.092	0.182	0.181	1.224
1.0	0.101	0.084	0.831	0.166	1.204
1.3	0.081	0.067	0.862	0.133	1.160
1.7	0.064	0.053	0.889	0.105	1.124
4.0	0.029	0.024	0.948	0.047	1.055
16	0.008	0.006	0.986	0.012	1.014
64	0.002	0.002	0.996	0.003	1.004
∞	0.0	0.0	1.0	0.0	1.0

The calculation of the mobility required the use of Equations (32) and (33). The result is,

$$V_f = \frac{be[v_1P_1(1+P_2)+v_2P_2(1+P_1)]}{1-P_1P_2} = \frac{b^2qE}{kT} \frac{[v_1P_1(1+P_2)+v_2P_2(1+P_1)]}{(1-P_1P_2)} = \mu E \quad (34)$$

where  $\mu$  is the mobility and  $E$  is the applied field. Therefore, with comparison with Equations (14) and (15),

$$\frac{kT\mu}{D} = \frac{q}{f} \quad (35)$$

This represented the mobility was proportional to the reciprocal of the correlation factor. This equation is a well known Einstein equation.

### Results and Discussion

In order to evaluate the effect of the vacancy being bound to the dislocation core, it is reasonable to simplify the model to reflect vacancy-core binding by introducing the single factor  $g^7$  to represent the ease of the

vacancy to escape from the core.

$$g = \exp(-Q/kT) \quad (36)$$

where  $Q$  is the vacancy-core binding energy.

The above  $g$  was substituted for the ratio of  $\omega_3$ , the vacancy escape frequency, to any other jump frequency. The above expressions of  $f$ ,  $D$ , and  $\mu$  were expressed in terms of  $g$  only and were summarized in Ref. 11. In Table 2, it is interesting that the limits of the mobility and diffusivity are so much in contrast to the correlation factor. The calculation of the tight binding model of a vacancy to an edge dislocation in an FCC crystal demonstrated some unexpected results<sup>12,13</sup>.

The limiting case of the vacancy tightly bound to the dislocation core is shown as  $g$  approaches zero. In this case,  $f$  also approaches zero since the tracer can go nowhere in one dimension with a vacancy mechanism. And diffusivity and the ratio of the mobility to the diffusivity become infinite in that limit. As Strak<sup>8</sup> stated, that the diffusivity becomes infinite in that limit is due to the abundance of vacancies in the core available to transport the tracer along the dislocation pipe. Clearly the same reason can not explain the ratio of the mobility to the diffusivity since they both have the same number of vacancies participating. The ratio of the mobility to the diffusivity increase without bounds because the length of the dislocation becomes infinite and a vacancy that moves the tracer parallel to the applied field may also move an infinite number of other solvent ions along the core in the process of arriving at the tracer. Thus, the so-called vacancy wind becomes infinite in the tight binding limit

At the contrast limit of vacancy repulsion from the core, no correlated motion,  $g$  becomes large, implying loose binding of the vacancy to the core and the limiting value of 1.0 for  $f$  is observed. For the diffusivity, it becomes zero. And  $kT$  times the ratio of the mobility to the diffusivity becomes one. In this limit, the calculation is approximate due to the definition of the configurations. However, the vacancy path away from the tracer does exist and this suggests that the limit is correct. Therefore, the correlation factor becomes one is perfectly understandable since only a single tracer-vacancy exchange will occur per vacancy. The diffusivity becomes zero because there are no available vaca-

ncies in that case, and  $kT$  times the ratio of the mobility to the diffusivity becomes unity since for every vacancy that does indeed move the tracer, it will do so with only one tracer jump.

Stark<sup>7</sup> applied this theory to explain the electro-migration-induced failure of metal interconnections in large-scale integrated circuits. Therein field-induced vacancy transports along dislocations and grain boundaries proceeds to a phase boundary. Then since the lattice diffusion coefficient is small because of the low homologous temperature, the vacancy flux forms voids which grow and decrease the conducting cross section. Joule heating results in an increased-void growth rate and ultimate failure is unavoidable. The mobility and diffusivity limits suggest that the phenomenon discussed by Stark<sup>8</sup> about vacancy tight binding to an edge dislocation simple cubic structure is not unique to the crystal structure but to the edge dislocation.

### Conclusions

1. The mobility in a field applied in  $+x$  direction was found to be  $kT\mu/D=q/f$ .

2. The correlation factor becomes zero as the ratio of the vacancy escape frequency to any other jump frequency,  $g$ , approaches zero, which violates the Einstein equation. However, the correlation factor becomes unity as expected with  $g$  approaching infinity.

3. As the correlation factor approaches zero, the diffusivity becomes infinity because the tracer jump frequency,  $\Gamma$ , increases to infinity faster than the correlation factor does to zero.

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