Modified Dechanneling Theory and Diffusion Coefficients

M. Kitagawa and Y. H. Ohtsuki

Department of Physics, Waseda University, Nishi-Ohkubo 4, Shinjuku, Tokyo, Japan

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A new type of dechanneling theory is presented by constructing a Fokker-Planck equation. The damping term, which is not renormalized to the diffusion coefficient, and a new term in addition to the usual diffusion equation appear in the Fokker-Planck equation. Making use of the general expression of the diffusion coefficient given by Ohtsuki, some simple analytic expressions for diffusion coefficients due to the many-phonon excitations, the one-electron excitation, and the plasmon excitation are presented.

I. INTRODUCTION

A rapidly growing interest has developed in the depth dependence of the channeling phenomenon, i.e., in the rate of dechanneling. A detailed knowledge of dechanneling, which consists of particle transition from the channeling motion inside the crystal to a random motion, gives information on the electronic distribution and on the ion-atom interaction potential. The axial dechanneling has been widely investigated for light ions in W,[1,2] Si,[3] and Ge[4,5] single crystals. The planar-dechanneling data[1,6,7] has been interpreted on the analogy of the axial-dechanneling theory.[7] Most dechanneling theories[4-10] are based on the diffusion-type equation first introduced by Lindhard,[8]

$$\frac{\partial g(\vec{p}_\perp, z)}{\partial z} = \text{div} D(\vec{p}_\perp)\, \text{grad} g(\vec{p}_\perp, z), \tag{1.1}$$

where $g(\vec{p}_\perp, z)d\vec{p}_\perp$ is the differential probability at the penetration depth z. $D(\vec{p}_\perp)$ is the diffusion coefficient which is calculated[8] from the "local" mean-square angular spread in the quasielastic approximation; i.e., for axial cases,

$$\left(\frac{\delta\Omega^2}{\delta z}\right)_n = \frac{d}{8E^2}\rho_\perp^2\left(\frac{K^2(r_\perp)}{r_\perp^2} + K'^2(r_\perp)\right) \tag{1.2}$$

for the one-phonon excitation and

$$\left(\frac{\delta\Omega^2}{\delta z}\right)_e = \frac{\pi Z_1^2 e^4}{E^2} L_e n(r_\perp) \tag{1.3}$$

for electronic excitations. In the above, E and $Z_1 e$ are the energy and the charge of the incident particle, respectively, $\rho_\perp^2$ is the mean-square amplitude of the thermal vibrations perpendicular to the string, and d is the interatomic distance along the row. $n(r_\perp)$ and $K(r_\perp)$ are the averaged electron-cloud density and the force acting on the ion at $r_\perp$ due to the string potential, respectively. L_e is defined as

$$L_e = \ln(2mv^2/I), \tag{1.4}$$

where m, v, and I are the electron mass, the ion velocity, and the mean ionization energy of the atom, respectively.

However, we note that the above theory has been introduced by some physical intuitions, and the intuitions bring forward too simplified an equation to interprete experimental data qualitatively. In this paper, we start from the Fokker-Planck equation taking into account the collision terms due to inelastic scattering and derive a modified diffusion equation. Damping effects due to inelastic scattering and the interaction between the two directional transversal scatterings are included in the modified equation. The exact expressions for the diffusion coefficient introduced in the modified diffusion equation are calculated for many-phonon excitations, the plasmon excitation, and the one-electron excitation both for axial and planar cases making use of the general expression of the "local" diffusion coefficients derived by Ohtsuki.[11]

II. MODIFIED DECHANNELING EQUATION

We consider a beam of positively charged particles incident in a low-index crystallographic direction. By multiple scattering with electrons and nuclei in the crystal, the transverse momentum of the channeled particle increases, and this leads to dechanneling.

Since, in our system, scattering processes are regarded as small-angle scatterings, the change of the distribution f of the channeled beam in phase space is described in terms of the generalized Fokker-Planck equation.

Let $\phi(\vec{r}_\perp, \vec{p}; \Delta\vec{p})$ be the transition probability of a collision in which the particle momentum $\vec{p}$ is changed to $\vec{p} + \Delta\vec{p}$ at the fixed point $\vec{r}_\perp = (x, y)$ in the plane perpendicular to the channeling axis z. By use of the transition probability ϕ, we obtain the generalized Fokker-Planck equation as follows:

$$\frac{\partial f}{\partial t} + \vec{v}\cdot\text{grad}_{\vec{r}}f - \text{grad}_{\vec{r}}U(r_\perp)\cdot\text{grad}_{\vec{p}}f$$

$$= -f\,\text{div}_{\vec{p}}\left(\left\langle\frac{\Delta\vec{p}}{\Delta t}\right\rangle\right) - \left\langle\frac{\Delta\vec{p}}{\Delta t}\right\rangle\cdot\text{grad}_{\vec{p}}f$$

$$+ \frac{1}{2} \sum_{i=x,y,z} \frac{\partial^2}{\partial p_i^2} \left(\left\langle \frac{\Delta p_i^2}{\Delta t} \right\rangle f \right)$$

$$+ \sum_{i<j} \frac{\partial^2}{\partial p_i \partial p_j} \left(\left\langle \frac{\Delta p_i \Delta p_j}{\Delta t} \right\rangle f \right)$$

$$+ O(\Delta p_i \Delta p_j \Delta p_k), \quad (2.1)$$

where $\langle \cdots \rangle$ means the averaged value over the transition probability ϕ, that is,

$$\left\langle \frac{\Delta \vec{p}}{\Delta t} \right\rangle = \int \frac{\Delta \vec{p}}{\Delta t} \, \phi(\vec{r}_\perp, \vec{p}; \Delta \vec{p}) d(\Delta \vec{p}). \quad (2.2)$$

In the above, $U(r_\perp)$ is the continuum potential and $\frac{1}{2} \langle \Delta p_i \Delta p_j / \Delta t \rangle = \sigma_{ij}$ is the $(i\text{-}j)$th element of the diffusion coefficient.

The relation between the energy transfor ΔE_i (the total energy transfer $\Delta E = \sum_i \Delta E_i$) and the momentum transfer Δp_i is written

$$\Delta E_i = (1/2M_1)(2p_i \Delta p_i + \Delta p_i^2), \quad (2.3)$$

where M_1 is the ion mass. From Eq. (2.3), it is easy to note that energy decrease (damping effect) may not be described in terms of Δp_i^2 (diffusion process), but in terms of Δp_i. If the damping force due to energy losses is directed against the particle's motion in our system, we can easily obtain

$$\langle \Delta \vec{p}/\Delta t \rangle \cong - S(r_\perp, E_z) \vec{p}/p_z, \quad (2.4)$$

where $S(r_\perp, E_z)$ is the stopping-power function[12-15] and $E \cong E_z$ the energy of ion.

In our system, σ_{zz} is not the usual diffusion coefficient. For the z component of scattering processes, energy losses $(\Delta E_z < 0)$ are dominant. Therefore, in the following, we neglect σ_{zz} because of $\langle \Delta p_z / \Delta t \rangle \gg \langle \Delta p_z^2 / \Delta t \rangle$.

We consider the axial case. In principle, from Eq. (2.1), it would be possible to determine physical quantities for dechanneling. This, however, meets considerable mathematical difficulties. Therefore, at first step, we restrict ourselves to the quasiequilibrium state,[8] where since channeled particles are mixed, it can be assumed that f is independent of x and y in the transversal region.[8,16] At the same time, in our case, we assume that time t is not explicitly contained in the distribution f. Taking into account that the continuum potential $U(x,y)$ is an even function both for x and y, and

$$z = \int_{E_z}^{E_0} \hat{S}^{-1}(E_z) dE_z,$$

Eq. (2.1) reduces to the differential equation in (p_x, p_y, E_z) space,

$$f = \frac{\hat{S}(E_0)}{\hat{S}(E_z)} \frac{E_0}{E_z} u, \quad (2.5a)$$

$$-\frac{\partial u}{\partial E_z} = \frac{1}{2E_z} (\vec{p}_\perp \cdot \text{grad}_{\vec{p}_\perp} u) + \frac{1}{\hat{S}(E_z) v_z}$$

$$\times \left(\sum_{i=x,y} \frac{\partial^2}{\partial p_i^2} (\hat{\sigma}_{ii} u) + 2 \sum_{i<j} \frac{\partial^2}{\partial p_i \partial p_j} (\hat{\sigma}_{ij} u) \right),$$

$$(2.5b)$$

where the caret over a symbol means the averaged value over the transversal region in an unit cell, that is, $\hat{S}(E_z)$ and $\hat{\sigma}_{ij}$ are the channeling stopping power and the channeling diffusion coefficient, respectively. E_0 is the incident ion energy.

Alternatively, we can write Eq. (2.5b) in the form of the cylindrical coordinate $(p_\perp, \theta, E_z)$. In the case discussed here, it is a good approximation that the distribution function u is isotropic in $(p_\perp, \theta)$ space. In this approximation, we can neglect cross terms of diffusion coefficients because of axial symmetry. From Eq. (2.5b), we obtain

$$-\frac{\partial u}{\partial E_z} = \frac{p_\perp}{2E_z} \frac{\partial u}{\partial p_\perp} + \frac{\partial^2}{\partial p_\perp^2} (\hat{\mu}_{\perp\perp} u)$$

$$+ \frac{1}{p_\perp} \frac{\partial}{\partial p_\perp} \{(2\hat{\mu}_{\perp\perp} - \hat{\mu}_{\theta\theta}) u\}, \quad (2.6)$$

where $\hat{\mu}_{\perp\perp}$ and $\hat{\mu}_{\theta\theta}$ are written using the usual diffusion coefficients $\hat{D}_{\perp\perp}$ and $\hat{D}_{\theta\theta}$,[17]

$$\hat{D}_{\perp\perp} = \frac{1}{2} \langle \Delta \hat{p}_\perp^2 / \Delta z \rangle = \hat{\mu}_{\perp\perp} \hat{S}(E_z),$$

$$\hat{D}_{\theta\theta} = \frac{1}{2} \langle \Delta \hat{p}_\theta^2 / \Delta z \rangle = \hat{\mu}_{\theta\theta} \hat{S}(E_z). \quad (2.7)$$

Strictly speaking, $\hat{\mu}_{\theta\theta}$ (or $\hat{D}_{\theta\theta}$) is not zero in our case, especially for the plasmon excitation. In random system, $\hat{\mu}_{\perp\perp} = \hat{\mu}_{\theta\theta}$ (or $\hat{D}_{\perp\perp} = \hat{D}_{\theta\theta}$). We note that the first term on the right-hand side of Eq. (2.6) is very small compared with the third term in our channeling condition where $\psi \lesssim \psi_c$ $(\psi = p_\perp/p_z$, ψ_c; the critical angle).

Thus, finally we have

$$-\frac{\partial u}{\partial E_z} = \frac{\partial^2}{\partial p_\perp^2} (\hat{\mu}_{\perp\perp} u) + \frac{1}{p_\perp} \frac{\partial}{\partial p_\perp} \{(2\hat{\mu}_{\perp\perp} - \hat{\mu}_{\theta\theta}) u\},$$

$$(2.8)$$

or for the steady-state process,

$$-\frac{\partial u}{\partial E_z} = \frac{1}{p_\perp} \frac{\partial}{\partial p_\perp} \left[p_\perp \hat{\mu}_{\perp\perp} \left(-\frac{d}{dp_\perp} \ln u_{eq} \right) u \right]$$

$$+ \frac{1}{p_\perp} \frac{\partial}{\partial p_\perp} \left(p_\perp \hat{\mu}_{\perp\perp} \frac{\partial u}{\partial p_\perp} \right), \quad (2.9)$$

where u_{eq} is the equilibrium distribution.

It is worth noting that for the steady-state process, $\hat{\mu}_{\theta\theta}$ does not appear in the differential equation. In Eq. (2.9), the second term in the right-hand side gives the usual diffusion equation widely used in dechanneling theories. For our case, we have from the standard potential,[8]

$$\frac{d}{dp_\perp} (\ln u_{eq}) = -\frac{p_\perp}{M_1} \frac{2}{E_z \psi_c^2} \frac{A \exp(2E_\perp / E_z \psi_c^2) + 1}{A \exp(2E_\perp / E_z \psi_c^2) - 1},$$

$$(2.10)$$

$$A = \frac{c^2 a^2}{r_0^2} + 1,$$

where a is the Thomas-Fermi screening length, πr_0^2 is the area of the unit mesh in the (x,y) plane, and $c \cong \sqrt{3}$, $E_\perp = p_\perp^2/2M_1$. From Eq. (2.10), we note that the first term of Eq. (2.9) is not neglected generally.

Now, the Fokker-Planck equation for axial case may be solved in principle only if we get the local stopping power and the local diffusion coefficient. Many authors[12-15] have already discussed the local stopping power. However, we have no calculation of the local diffusion coefficient except for simple derivations according to the Lindhard theory.[8]

Recently, according to the steady-increase model, Björkqvist et al.[18] calculated dechanneled fractions taking into account the damping effect.[8] In our theory, the damping effect are introduced in $\langle \Delta \vec{p}/\Delta t \rangle$ [Eq. (2.4)], which does not appear in the usual diffusion equation.

Dechanneling rate α per unit energy loss is defined as

$$\alpha = \frac{1}{F}\frac{\partial F}{\partial E_z}, \qquad (2.11)$$

where

$$F = \int_0^{p_{\perp c}} f 2\pi p_\perp \, dp_\perp, \quad p_{\perp c} = p_z \psi_c.$$

From Eqs. (2.5a) and (2.11), the damping part α_{da} of dechanneling rate α is obtained:

$$\alpha_{da} = -\frac{1}{E_z} - \frac{1}{\hat{S}(E_z)}\frac{d\hat{S}(E_z)}{dE_z}. \qquad (2.12)$$

The longitudinal- and the transverse-energy losses are included in Eq. (2.12). Equation (2.12) shows that the contribution of the damping effects becomes remarkable at low-energy regions (see Sec. V).

III. DIFFUSION COEFFICIENTS FOR PHONON EXCITATIONS

In this and the following sections, we calculate the local diffusion coefficients introduced in Sec. II, from the general expression derived by Ohtsuki,[11]

$$\left\langle \frac{\Delta p_i^2}{\Delta z} \right\rangle = \frac{1}{4\pi^2 v_z^2} \int \sum_{h_\perp} q_i^2 S(\vec{q}, \vec{q}+\vec{h}_\perp) e^{i\vec{h}_\perp \cdot \vec{r}_\perp} d\vec{q}, \qquad (3.1)$$

where $S(\vec{q}, \vec{q}+\vec{h}_\perp)$ is the inelastic scattering factor with Umklapp process corresponding to the two-dimensional reciprocal-lattice vector $\vec{h}_\perp$. For convenience sake, momentum transfer $\Delta \vec{p}$ from the initial momentum $\hbar K_z = p_z$ is written as $\hbar \vec{q}$ on the right-hand side of Eq. (3.1). For phonon excitations, $S(\vec{q}, \vec{q}+\vec{h}_\perp)$ is given as[19]

$$S(\vec{q}, \vec{q}+\vec{h}_\perp) = \frac{1}{V_{cell}} v_{\vec{q}} v_{\vec{q}+\vec{h}_\perp}$$

$$\times (e^{-M(\vec{h}_\perp)} - e^{-M(\vec{q})-M(\vec{q}+\vec{h}_\perp)})$$

$$\times \delta\left(|\vec{K}_z + \vec{q}| - K_z + \frac{\Delta E}{\hbar v_z}\right), \qquad (3.2)$$

where $v_{\vec{q}}$ and $e^{-M(\vec{q})}$ are the usual scattering factor and the Debye-Waller factor, respectively. V_{cell} means the volume of the unit cell. The diffusion coefficient D introduced in above section is related by

$$D_{ij} = \tfrac{1}{2}\langle \Delta p_i^2/\Delta z \rangle. \qquad (3.3)$$

First, we try to derive the Lindhard expression (1.2) for the diffusion coefficient due to phonon excitation from our exact expression (3.1). When we consider the one-phonon excitation, the Debye-Waller factor $e^{-M(\vec{q})}$ is expanded up to the second power for $M(\vec{q}) \equiv \tfrac{1}{4}\rho_\perp^2 q^2$, and we obtain

$$\left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle = \frac{\rho_\perp^2}{16\pi^2 v_z^2}\frac{1}{V_{cell}} \int \sum_h q_\perp^2 v_{\vec{q}}\, v_{\vec{q}+\vec{h}_\perp}$$

$$\times \{\vec{q}^2 + (\vec{q}+\vec{h}_\perp)^2 - \vec{h}_\perp^2\}$$

$$\times e^{i\vec{h}_\perp \cdot \vec{r}_\perp} \delta\left(|\vec{K}_z + \vec{q}| - K_z + \frac{\Delta E}{\hbar v_z}\right) d\vec{q}. \qquad (3.4)$$

If we assume that the phonon scattering is described only on the plane perpendicular to the channeling axis, we have

$$\left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle = \frac{\rho_\perp^2}{8\pi^2 v_z^2}\frac{1}{V_{cell}} \int \sum_h q_\perp^2 (\vec{q}_\perp^2 + \vec{q}_\perp \cdot \vec{h}_\perp) V_{\vec{q}_\perp} V_{\vec{q}_\perp + \vec{h}_\perp}$$

$$\times e^{i\vec{h}_\perp \cdot \vec{r}_\perp} \delta\left(|\vec{K}_z + \vec{q}| - K_z + \frac{\Delta E}{\hbar v_z}\right) d\vec{q}, \qquad (3.5)$$

where $\vec{q}_\perp$ is the scattering vector on the plane and $V_{\vec{q}_\perp}$ means the two-dimensional component $(q_z = 0)$ of the scattering factor:

$$V_{\vec{q}_\perp} \equiv v_{\vec{q}}\big|_{q_z=0}. \qquad (3.6)$$

If we consider the continuum potential to be[20]

$$V(\vec{r}_\perp) = \sum_{q_\perp} V_{\vec{q}_\perp} e^{-i\vec{q}_\perp \cdot \vec{r}_\perp}, \qquad (3.7)$$

it is easy to show that the expression (3.5) coincides with the Lindhard expression (1.2).

However, we have to point out that some approximations assumed above in deriving the Lindhard expression are not so good. Back scatterings by many phonon excitations are also important.

Now we show that another approximation gives a reasonable expression for the diffusion coefficient due to many phonon excitations. We do not expand the Debye-Waller factor, which means that we consider many-phonon excitations, and we neglect the second term in Eq. (3.2). This assumption is valid only if the incident energy of ions is much larger and $|\vec{q}| \gg |\vec{h}_\perp|$. Thus we obtain for axial cases

$$\left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle = \frac{1}{4\pi v_z^2} \frac{1}{V_{cell}} \int \sum_{h_\perp} q_\perp^2 v_{\vec q}^2 \; v_{\vec q + \vec h_\perp}^* e^{-M(\vec h_\perp)} e^{i\vec h_\perp \cdot \vec r_\perp}$$

$$\times \delta\left(|\vec K_z + \vec q| - K_z + \frac{\Delta E}{\hbar v_z} \right) d\vec q$$

$$\cong \left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle_{random} P(\vec r_\perp), \tag{3.8}$$

where $\langle \Delta p_\perp^2/\Delta z \rangle_{random}$ is the diffusion coefficient in random case given by Bohr,[21]

$$\left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle_{random} = \frac{8\pi Z_1^2 Z_2^2 e^4 N}{v_z^2} L_n, \tag{3.9}$$

and $P(\vec r_\perp)$ is the distribution function of the atom in thermal motion at the (x, y) plane,

$$P(\vec r_\perp) = \sum_{h_\perp} e^{-M(\vec h_\perp)} e^{i\vec h_\perp \cdot \vec r_\perp} = \frac{r_0^2}{\rho_\perp^2} \exp\left(-\frac{r_\perp^2}{\rho_\perp^2} \right). \tag{3.10}$$

In the above,

$$L_r \cong \ln\left(1.29 \frac{aE_z}{Z_1 Z_1 e^2} \frac{M_2}{M_1 + M_2} \right),$$

and M_2 and Z_2 are the mass and the atomic number of the atom.

The expression (3.8) means that the momentum deviation is caused by Rutherford scatterings at atoms located in the thermal distribution.

Diffusion coefficients for the planar case are also derived from Eq. (3.1) with same assumptions taking into account $\vec h_\perp = (0, h_y)$,

$$\langle \Delta p_y^2/\Delta z \rangle = \langle \Delta p_y^2/\Delta z \rangle_{random} P(y), \tag{3.11}$$

where $P(y)$ is the distribution function of the atom at y from the channeling plane,

$$P(y) = \frac{d_y}{(2\pi)^{1/2}\rho_y} \exp\left(-\frac{y^2}{2\rho_y^2} \right), \tag{3.12}$$

where ρ_y means the root-mean-square amplitude of the lattice vibration orthogonal to the channeling plane, and d_y is the distance between channeling planes.
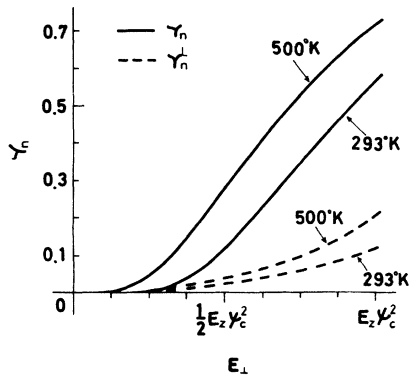

FIG. 1. Comparison of γ_n and γ_n^L as a function of $E_\perp$ for 1.5-MeV ^{1}H$^+$ in the Ge $\langle 100 \rangle$ axis.
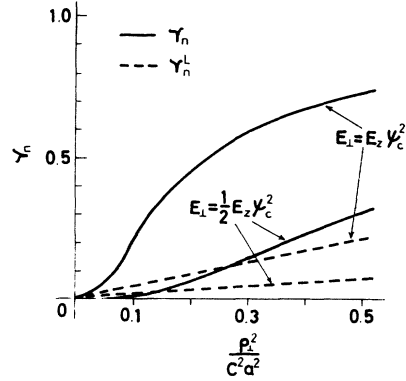

FIG. 2. Temperature dependence of γ_n and γ_n^L for 1.5-MeV ^{1}H$^+$ in the Ge $\langle 100 \rangle$ axis.

It is noted that for planar case, D_{xx} becomes zero in the theory used by Campisano et al.,[7] but in our theory, we have $D_{xx}(y, E_z) \neq 0$.

Numerical calculations of diffusion coefficients due to the many phonon excitations for axial case performed by use of the local diffusion coefficients, Eq. (3.8),

$$D_{\perp\perp}(E_\perp, E_z) = D_{random} \gamma_n, \tag{3.13}$$

where

$$\gamma_n = \exp\left\{ -\frac{c^2 a^2}{\rho_\perp^2} \left[\exp\left(\frac{2E_\perp}{E_z \psi_c^2} \right) - 1 \right]^{-1} \right\}.$$

In Fig. 1 we plot γ_n as the function of $E_\perp$, compared with the Lindhard's factor γ_n^L of the one-phonon excitation, for 1.5-MeV ^{1}H$^+$ in Ge It is evident that factors γ_n and γ_n^L are coincident at small $E_\perp$ region, but not at larger region of $E_\perp$.

We also show in Fig. 2 the temperature dependence of γ_n and γ_n^L at the same condition, as a function of $\rho_\perp^2/c^2 a^2$.

IV. ELECTRONIC EXCITATIONS

It is important to consider the plasmon excitation when we calculate diffusion coefficients, besides the one-electron excitations. Although the angular spread corresponding to K_c^2 (K_c being the cutoff wave number of the plasmon) is very small compared with that of Rutherford scattering, the transition probability for plasmon excitations is very large. Then, we have to consider the plasmon excitation in the calculation of the diffusion coefficient.

A. Plasmon Excitations

When we take the electron-gas model, plasmon excitations are homogeneous. Then, we need not distinguish the axial and planar cases.

In random-phase approximation of plasmon excitation, $S(\vec q, \vec q + \vec h) = S(\vec q, \vec q) \delta_{h,0}$ in Eq. (3.1) is de-

rived as[22]

$$S(\vec{q}, \vec{q}) = \frac{4Z_1 e^2 \hbar v_s}{q_\perp^2 + q_s^2} \ \mathrm{Im}\left(\frac{-1}{\epsilon(\vec{q}_\perp, q_s)}\right) , \qquad (4.1)$$

where $\epsilon(\vec{q}_\perp, q_s)$ is the complex dielectric constant for the electron gas. Inserting Eq. (4.1) with

$$\mathrm{Im}\left(\frac{-1}{\epsilon(\vec{q}_\perp, q_s)}\right) \cong \mathrm{Im}\left(\frac{-1}{\epsilon(0, q_s)}\right) = \frac{\pi \omega_p}{2v_s} \ \delta\left(q_s - \frac{\omega_p}{v_s}\right) ,$$

$\hbar\omega_p$ being the plasmon energy, we obtain

$$\left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle = \frac{Z_1 e^2 \hbar \omega_p}{2v_s^2} \left\{ K_c^2 - \left(\frac{\omega_p}{v_s}\right)^2 \ln\left[\left(\frac{K_c v_s}{\omega_p}\right)^2 + 1\right]\right\} . \qquad (4.2)$$

When we consider the high-energy case

$$v_s^2 \gg (\omega_p/K_c)^2, \qquad (4.3)$$

we may derive

$$\left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle = \frac{Z_1 e^2 \hbar \omega_p K_c^2}{2v_s^2} . \qquad (4.4)$$

Since $\omega_p \sim n_v^{1/2}$ and $K_c = 0.47 r_s^{1/2} K_F \sim n_v^{1/3}$ (n_v is the valence electron density), $\langle \Delta p_\perp^2/\Delta z \rangle$ is proportional to $n_v^{7/6}$. Thus, it is roughly valid that $\langle \Delta p_\perp^2/\Delta z \rangle$ is proportional to n_v. At the end of this section, we compare Eq. (4.4) with that of one-electron excitation.

B. One-Electron Excitation

Core and valence electrons are also excited by ion motion independently (not collective as the plasmon). In this case, $S(\vec{q}, \vec{q} + \vec{h}_\perp)$ in Eq. (3.1) is written[23]

$$\frac{1}{V_{\mathrm{cell}}} v_{\vec{q}}^* v_{\vec{q}+\vec{h}_\perp} \left\{\sum_i f_{ii}(\vec{h}_\perp) - \sum_{i,j} f_{ij}(\vec{q}+\vec{h}_\perp) f_{ij}(\vec{q})\right\}$$

$$\times \delta\left(|\vec{K}_s + \vec{q}| - K_s + \frac{I}{\hbar v_s}\right) , \qquad (4.5)$$

where $f_{ij}(\vec{q})$ is defined by the wave function $\phi_i(\vec{R})$ of the atomic electrons

$$f_{ij}(\vec{q}) = \int \phi_i^*(\vec{R}) e^{-i\vec{q}\vec{R}} \phi_j(\vec{R}) d\vec{R}. \qquad (4.6)$$

Then diffusion coefficients in our case obtained as, for the axial case,

$$\left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle = \frac{1}{4\pi^2 v_s^2 V_{\mathrm{cell}}} \int \sum_{h_\perp} q_\perp^2 v_{\vec{q}}^* v_{\vec{q}+\vec{h}_\perp}$$

$$\times \left(\sum_i f_{ii}(\vec{h}_\perp) - \sum_{i,j} f_{ij}(\vec{q}+\vec{h}_\perp) f_{ij}(\vec{q})\right)$$

$$\times e^{i\vec{h}_\perp \cdot \vec{r}_\perp} \delta\left(|\vec{K}_s + \vec{q}| - K_s + \frac{I}{\hbar v_s}\right) d\vec{q},$$

and for the planar case $\qquad (4.7)$

$$\left\langle \frac{\Delta p_y^2}{\Delta z} \right\rangle = \frac{1}{4\pi v_s^2 V_{\mathrm{cell}}} \int \sum_{h_y} q_y^2 v_{\vec{q}}^* v_{\vec{q}+h_y}$$

$$\times \left(\sum_i f_{ii}(h_y) - \sum_{i,j} f_{ij}(\vec{q}+h_y) f_{ij}(\vec{q})\right)$$

$$\times e^{i h_y \cdot y} \delta\left(|\vec{K}_s + \vec{q}| - K_s + \frac{I}{\hbar v_s}\right) d\vec{q}. \qquad (4.8)$$

For the high-energy case, the second term in Eq. (4.7) and Eq. (4.8), $f_{ij}(\vec{q}+\vec{h}_\perp) f_{ij}(\vec{q})$, is also neglected, as in the case of phonon excitation. In this case, Eqs. (4.7) and (4.8) are written, for the axial case,

$$\left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle = \frac{1}{4\pi^2 v_s^2 V_{\mathrm{cell}}} \int \sum_i \sum_{h_\perp} q_\perp^2 v_{\vec{q}} \ v_{\vec{q}+\vec{h}_\perp} f_{ii}(\vec{h}_\perp)$$

$$\times e^{i\vec{h}_\perp \cdot \vec{r}_\perp} \delta\left(|\vec{K}_s + \vec{q}| - K_s + \frac{I}{\hbar v_s}\right) d\vec{q}, \qquad (4.9)$$

and for the planar case

$$\left\langle \frac{\Delta p_y^2}{\Delta z} \right\rangle = \frac{1}{4\pi^2 v_s^2 V_{\mathrm{cell}}} \int \sum_i \sum_{h_y} q_y^2 v_{\vec{q}} \ v_{\vec{q}+h_y} f_{ii}(h_y)$$

$$\times e^{i h_y \cdot y} \delta\left(|\vec{K}_s + \vec{q}| - K_s + \frac{I}{\hbar v_s}\right) d\vec{q}. \qquad (4.10)$$

If the $\vec{h}_\perp$ dependence of the scattering factor $v_{\vec{q}+\vec{h}_\perp}$ is neglected in Eqs. (4.9) and (4.10), we obtain, for example, for the axial case

$$\left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle \cong \frac{4\pi Z_1^2 e^4}{v_s^2} L_e n(r_\perp) \qquad (4.11)$$

and for the planar case

$$\left\langle \frac{\Delta p_y^2}{\Delta z} \right\rangle \cong \frac{4\pi Z_1^2 e^4}{v_s^2} L_e n(y), \qquad (4.12)$$
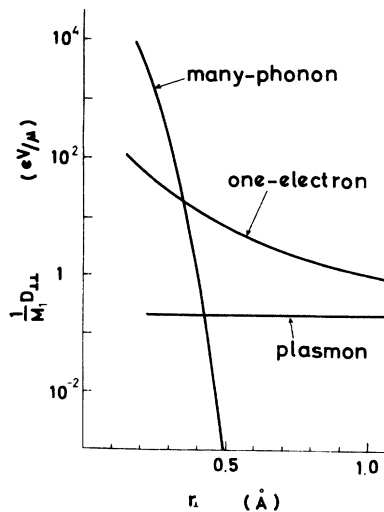

FIG. 3. Relative contributions of many-phonon, plasmon, and one-electron excitations to diffusion coefficients $(1/M_1)D_{\perp\perp}$ as a function of the distance $r_\perp$ from the string for 1.5-MeV ^{1}H$^+$ in the Ge $\langle 100 \rangle$ axis at 293 °K.

TABLE I. Dechanneling rate for 1.5-MeV $^1H^+$, $^2D^+$, and $^4He^+$ ions in the Ge $\langle 100 \rangle$ axis at room temperature in units of 10^{-6} eV^{-1}. α_{expt} and α_M mean the experimental value of the dechanneling rate and Morita's quasiempirical result, respectively (Ref. 5). α_{da} means the damping part of dechanneling rate.

	α_{expt}	α_M	$\alpha_M + \alpha_{da}$
$^1H^+$	5.4 ± 0.2	5.90	5.60
$^2D^+$	2.9 ± 0.1	3.22	2.82
$^4He^+$	0.84 ± 0.04	1.97 (He$^+$)	1.23 (He$^+$)
		0.99 (He^{2+})	0.30 (He^{2+})

since

$$\frac{1}{V_{cell}} \sum_{\vec{h}_\perp} \sum_i f_{ii}(\vec{h}_\perp) e^{i\vec{h}_\perp \cdot \vec{r}_\perp} = n(r_\perp) ,$$

and so on. In the quasielastic approximation, Eq. (4.11) coincides with the Lindhard expression [Eq. (1.3)].

Here we compare the plasmon diffusion coefficient [Eq. (4.4)] with the one-electron diffusion coefficient [Eq. (4.11)]:

$$\frac{\langle \Delta p_\perp^2 / \Delta z \rangle_{one-el}}{\langle \Delta p_\perp^2 / \Delta z \rangle_{plas}} \simeq \frac{4 E_F Z_1 L_e}{\hbar \omega_p} , \qquad (4.13)$$

where E_F is the Fermi energy and $E_F \sim \hbar \omega_p$ in usual metals.

Using the electron density in the atom by the Moliére formula,[24] numerical calculations of Eqs. (3.8), (4.4), and (4.11) are performed for 1.5-MeV $^1H^+$ in the Ge $\langle 100 \rangle$ axis and shown in Fig. 3. As is shown in Eq. (4.13), the plasmon diffusion coefficient is of the same order with the one-electron diffusion coefficient at larger $r_\perp$. It is worth noting that the plasmon diffusion coefficient is not proportional to the stopping power due to the plasmon excitation.

V. CONCLUDING REMARKS

A new type dechanneling theory was developed by constructing the Fokker-Planck equation. A damping term and a new term in addition to the usual diffusion equation appear in the Fokker-Planck equation, which are not neglected in general. The Fokker-Planck equation includes the local stopping power and the local diffusion coefficients.

Making use of the general expression of the local diffusion coefficient given by Ohtsuki, we calculated the many-phonon excitation, the one-electron excitation, and the plasmon excitation. Simple expressions of the diffusion coefficients of Lindhard were confirmed critically with the understanding that Lindhard's expressions are rough. However, we have to point out that our simple analytical expressions for many-phonon excitations [Eq. (3.8)] and the one-electron excitation [Eq. (4.11) or Eq. (4.12)] are also rough estimations, though the expression due to the plasmon excitation [Eq. (4.4)] is exact. It is serious that we neglected the $h_\perp$ dependence of the scattering factor $v_{\vec{q}+\vec{h}_\perp}$. Exact calculations of diffusion coefficients due to phonon excitations [Eqs. (3.1) and (3.2)] and due to one-electron excitations [Eqs. (4.7) and (4.8)] are now in progress.

Equation (2.12) shows that the contribution of the damping effect is of the same order with the experimental values of dechanneling rate[5]; i.e., the order of the experimental value of dechanneling rate is about 10^{-6}–10^{-7} eV^{-1} for 1.5-MeV $^1H^+$, $^2D^+$, and $^4He^+$ in the Ge $\langle 100 \rangle$ channel. For example, making comparison with the experiment mentioned above, damping effects contribute about 7% and 15% for the respective cases of $^1H^+$ and $^2D^+$, and more remarkable for the case of He ion (see Table I). In Table I, α_M means Morita's quasiempirical result,[5] in which the damping effect is not taken into account. Therefore, at this stage, we come to the conclusion that the damping effect may not be neglected for dechanneling, especially where the ion-mass effect is concerned.

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