

*Multiple Scattering of Channeled Ions in Crystals*

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The Fokker-Planck equation for scattering of channeled ions by electrons or thermal vibrations of lattice atoms is derived. Solutions of the equations for a number of cases of interest are obtained. An analysis of dechanneling experiments is carried out.

1. INTRODUCTION

THE channeling effect is finding increasing applications in solid state, nuclear, and atomic physics<sup>[1,2]</sup>. The classical theory of channeling was developed by Lindhard<sup>[3]</sup> and by Erginsoy et al.<sup>[4]</sup>. Kagan and Kononets<sup>[5]</sup> used the density-matrix formalism to describe the channeling effect and, in particular, to elucidate the quantum and classical aspects of this phenomenon. Kalashnikov, Ryazanov, and Chukhnovskii<sup>[6]</sup> investigated the spatial regrouping of particles in channeling. It follows from the listed references that channeled ions do not pass close to the atomic nuclei. Therefore the cross sections of the different physical reactions are significantly altered by channeling of the ions. Owing to the scattering of the ions by electrons, thermal vibrations, defects, etc., the transverse energy of the ion increases and the ion leaves the channel. Experiments have shown that the dechanneling is quite intense. For a large group of problems connected with the use of the channeling effect, it is necessary to know the rate of departure of the ions from the channel. The purpose of the present paper is to consider this problem.

We shall consider mainly multiple scattering of heavy charged particles (protons,  $\alpha$  particles, ions) by electrons and in part also by thermal vibrations of atoms. As is well known<sup>[7]</sup>, classical theory makes it possible in this case to explain all the experiments performed to date. We shall therefore use the classical description of the motion of particles in a crystal. We consider axial channeling. The distribution of the electron density in the channel is described on the basis of the Thomas-Fermi model of the atom and of the free-electron model.

2. ION DECHANNELING IN THE THOMAS-FERMI MODEL

Since the increment  $\delta E_{\perp}$  of the transverse energy is small in comparison with  $E_{\perp}$  in Coulomb scattering described by the Rutherford formula, we shall use the Fokker-Planck formula to study the behavior of channeled ions scattered by crystal atoms. We assume also that the crystal is thick enough to be able to average over all the impact parameters of the collision between the ion and a chain of atoms, or, in other words, to establish an equilibrium microcanonical distribution in the transverse plane<sup>[4]</sup>, when the ion can be observed with equal probability at any point of the accessible

region  $U(\mathbf{r}) \leq E_{\perp}$ , where  $E_{\perp} = \frac{1}{2}Mv_{\perp}^2 + U(\mathbf{r})$  is the total energy of transverse motion and  $U(\mathbf{r})$  is the potential energy of the ion in the field of the chain of atoms. The Fokker-Planck equation for the distribution function  $f(E, E_{\perp}, x)$  takes the following form ( $E$  is the total energy of the ion and  $x$  is the depth of penetration):

$$\frac{\partial f}{\partial x} = -\frac{\partial}{\partial E_{\perp}} \left( \left\langle \frac{\Delta E_{\perp}}{\Delta x} \right\rangle f \right) + \frac{1}{2} \frac{\partial^2}{\partial E_{\perp}^2} \left( \left\langle \frac{\Delta E_{\perp}^2}{\Delta x} \right\rangle f \right) - \frac{\partial}{\partial E} \left( \left\langle \frac{\Delta E}{\Delta x} \right\rangle f \right), \tag{1}$$

where the averaging  $\langle \dots \rangle$  is carried out over the accessible region.

Let us consider, for example, scattering by electrons. Since  $E_{\perp} = E\theta^2 + U(\mathbf{r})$  at small angles between the velocity  $\mathbf{v}$  and the channel axis  $\mathbf{x}$ , it follows that

$$\Delta E_{\perp} = E\Delta\theta^2. \tag{2}$$

In scattering through an angle  $\epsilon$  we have

$$\cos \theta' = \cos \theta \cos \epsilon + \sin \theta \sin \epsilon \cos \varphi, \tag{3}$$

where  $\varphi$  is the angle between the scattering plane and the plane passing through the directions of  $\mathbf{v}$  and  $\mathbf{x}$ ;  $\theta'$  is the angle between the new position of the velocity vector  $\mathbf{v}'$  and the  $\mathbf{x}$  axis. This yields for small  $\theta$  and  $\epsilon$

$$(\theta')^2 - \theta^2 = \epsilon^2 - 2\theta\epsilon \cos \varphi \tag{4}$$

and

$$\Delta E_{\perp} = E(\epsilon^2 - 2\theta\epsilon \cos \varphi) \tag{5}$$

$$\Delta E_{\perp}^2 = E^2 4\theta^2 \epsilon^2 \cos^2 \varphi \tag{6}$$

accurate to quantities of order  $\epsilon^2$ . Averaging over the probability of scattering along the path  $\Delta x$ :

$$dW = 2\pi\sigma(\epsilon) \sin \epsilon d\epsilon \rho \Delta x,$$

where  $\sigma(\epsilon)$  is the differential scattering cross section, we obtain, at a density  $\rho$  of the scattering centers (electrons), the average increment of the transverse energy per unit length

$$\Delta E_{\perp} / \Delta x = E \overline{\Delta \epsilon^2} / \Delta x \tag{7}$$

and the mean squared increment of the transverse energy

$$\Delta E_{\perp}^2 / \Delta x = 2E^2 \theta^2 \overline{\Delta \epsilon^2} / \Delta x,$$

or, after substituting the kinetic energy of the transverse motion  $E\theta^2 = E_{\perp} - U(\mathbf{r})$ ,

$$\Delta E_{\perp}^2 / \Delta x = 2E(E_{\perp} - U(\mathbf{r})) \overline{\Delta \epsilon^2} / \Delta x, \tag{8}$$

where

$$\overline{\Delta \varepsilon^2} = 2\pi\rho\Delta x \int \varepsilon^2 \sigma(\varepsilon) \sin \varepsilon d\varepsilon \quad (9)$$

$$\langle \Delta \varepsilon_{\perp}^2 / \Delta x \rangle_e = B\varepsilon_{\perp} \bar{\nu}, \quad (16)$$

is the mean squared scattering angle.

Averaging over the admissible region (which is equivalent to averaging over a  $\Delta x$  containing  $\sim 1000$  atomic layers) is carried out by means of the formula

$$\langle \Delta E_{\perp} \rangle = \frac{1}{\pi(r_0^2 - r_1^2)} \int_{r_1}^{r_0} \Delta E_{\perp} 2\pi r dr \quad (10)$$

and similarly for  $\Delta E_{\perp}^2$  and  $\Delta E$ , where  $r_0 = 1/\pi Nd$ ,  $N$  is the density of the atoms,  $d$  is the distance between the atoms of the given chain, and  $r_1$  is determined from the condition  $E_{\perp} = U(r_1) - U(r_0)$ , i.e.,  $r_1$  is the distance of the shortest approach of the ion to the atom chain. It is seen from (7) and (8) that

$$\frac{1}{2} \left\langle \frac{\Delta E_{\perp}^2}{\Delta x} \right\rangle = \left\langle \frac{\Delta E_{\perp}}{\Delta x} [E_{\perp} - U(r)] \right\rangle. \quad (11)$$

From this we have at  $r_0 \gg r_1$ , when the dimension of the averaging region is constant,

$$\left\langle \frac{\Delta E_{\perp}}{\Delta x} \right\rangle \approx \frac{1}{2} \frac{\partial}{\partial E_{\perp}} \left\langle \frac{\Delta E_{\perp}^2}{\Delta x} \right\rangle. \quad (12)$$

Thus, without taking into account the deceleration at  $r_0 \gg r_1$ , the Fokker-Planck equation goes over into the diffusion equation

$$\frac{\partial f}{\partial x} = \frac{1}{2} \frac{\partial}{\partial E_{\perp}} \left\langle \frac{\Delta E_{\perp}^2}{\Delta x} \right\rangle \frac{\partial f}{\partial E_{\perp}}, \quad (13)$$

and a more general expression, when we cannot assume that  $r_0 \gg r_1$ , is (it is derived in the Appendix):

$$\frac{\partial f}{\partial x} = \frac{1}{2S(E_{\perp})} \frac{\partial}{\partial E_{\perp}} \left( S(E_{\perp}) \left\langle \frac{\Delta E_{\perp}^2}{\Delta x} \right\rangle \frac{\partial f}{\partial E_{\perp}} \right), \quad (13')$$

where  $S(E_{\perp})$  is the area of the accessible region.

For a standard Thomas-Fermi potential<sup>[3]</sup>

$$U(r) = \frac{Z_1 Z_2 e^2}{d} \ln \left( 1 + \frac{3a^2}{r^2} \right)$$

where  $a$  is the screening constant and  $Z_1$  and  $Z_2$  are the atomic numbers of the particle and of the lattice atom, we have

$$E_{\perp} = \frac{Z_1 Z_2 e^2}{d} \ln \frac{1 + 3a^2/r_1^2}{1 + 3a^2/r_0^2}$$

We shall henceforth replace  $E_{\perp}$  by the dimensionless transverse energy

$$\varepsilon_{\perp} = Ed(Z_1 Z_2 e^2)^{-1} = 2E_{\perp} (E\psi_1^2)^{-1},$$

where  $\psi_1$  is Lindhard's critical channeling angle. By using the mean squared scattering angle for scattering of fast ions by atomic electrons

$$\overline{\Delta \varepsilon^2} = \frac{m}{2ME} S_e \rho \Delta x, \quad (14)$$

where  $S_e$  is the decelerating ability of one atomic electron:

$$S_e = \frac{4\pi Z_1^2 e^4 L_e}{mv^2}, \quad L_e = \ln \frac{2mv^2}{I},$$

$I$  is the average ionization potential, and the electron density  $\rho$  is given by

$$\rho = \frac{1}{4\pi Z_1 e} \frac{d(rU')}{dr},$$

we obtain from (10)

$$\langle \Delta \varepsilon_{\perp} / \Delta x \rangle_e = \frac{B}{A} F, \quad (15)$$

where

$$A = 1 + 3a^2/r_0^2, \quad B = Z_1 \pi e^2 Nd L_e / E,$$

$$F = 1 - A^{-1} \exp(-\varepsilon_{\perp}),$$

$$\bar{\nu} = \frac{F}{A} \left[ 1 + \frac{A}{2\varepsilon_{\perp}} \left( \frac{\varepsilon_{\perp}(1-F)}{1-A+AF} - 1 \right) \right]. \quad (17)$$

According to Lindhard<sup>[3]</sup>, the average change of the transverse energy  $\langle \Delta \varepsilon_{\perp} / \Delta x \rangle_{th}$  (th stands for thermal) due to scattering by the vibrating atoms is

$$\left\langle \frac{\Delta \varepsilon_{\perp}}{\Delta x} \right\rangle_{th} = \frac{B\kappa F}{1-A+AF} \left[ F^3 \left( \frac{2}{3} + \frac{1}{1-F} \right) - \left( 1 - \frac{1}{A} \right)^3 \left( \frac{2}{3} + A \right) \right], \quad (18)$$

where  $\kappa = Z_2 \rho_{\perp}^2 (3a^2 L_e)^{-1}$  and  $\rho_{\perp}$  is the rms transverse displacement of the atom for thermal vibrations.

We consider now the change of the transverse energy due to deceleration of the particles. Assuming that

$$\frac{dE}{dx} = S_e [(1-\alpha)NZ_2 + \alpha\rho], \quad (19)$$

where  $\alpha$  is the coefficient for the separation of the energy losses into losses due to short-range and long-range collisions, and averaging over the accessible region, we obtain

$$\left\langle \frac{\Delta \varepsilon_{\perp}}{\Delta x} \right\rangle_{dec} = -\frac{M}{m} B\psi_1^2 \varepsilon_{\perp} \{ (1-\alpha)\beta + \alpha\bar{\nu} \}, \quad (20)$$

$$\beta = 1 - \frac{F(A-1)}{\varepsilon_{\perp}(1-A+AF)} [A - \ln(A-1) - (F^{-1}-1)(\varepsilon_{\perp} + \ln A) + \ln F]. \quad (21)$$

From (20) and (15) we find that the increase of the transverse energy  $\langle \Delta \varepsilon_{\perp} / \Delta x \rangle_e$  exceeds its decrease due to deceleration,  $\langle \Delta \varepsilon_{\perp} / \Delta x \rangle_{dec}$ , when

$$M\psi_1^2 / m < F / A\varepsilon_{\perp} \{ (1-\alpha)\beta + \alpha\bar{\nu} \}. \quad (22)$$

It is obvious that the lower limit of the right-hand side is equal to two, since the upper limit of the curly bracket is unity, and  $A \approx 1$ . We see therefore that for fast ions, when  $M\psi_1^2 / m \lesssim 2$ , the decrease of  $E_{\perp}$  due to deceleration can be neglected. In the opposite case, when the condition (22) is not satisfied, pulling of the atoms towards the channel axis is possible.

Averaging (19) over the accessible region, we obtain

$$\left\langle \frac{\Delta E}{\Delta x} \right\rangle = -\frac{M}{m} B E \psi_1^2 \left[ 1 - \alpha + \frac{\alpha F}{A} \right]. \quad (23)$$

We see that the Fokker-Planck equation (1) cannot be solved analytically with the obtained coefficients. We shall, however, make a number of estimates in Sec. 4 on the basis of the Thomas-Fermi model of the atom.

### 3. DECHANNELING OF IONS BY SCATTERING BY ELECTRONS

When the ion beam is directed along the channel axis, most ions are localized in the central part of the channel. The electron density in the central part of the channel is produced in the case of metals by free electrons. As shown by Appleton et al.<sup>[4]</sup>, even in the case of silicon the electron density is due mainly to the four valence electrons and is homogeneous with high accuracy ( $\sim 5-10\%$ ). Moreover, the energy losses of the channeled ions are due mainly to deceleration by the free and valence electrons<sup>[4,8]</sup>. It is therefore

reasonable to consider dechanneling of the ions as a result of the scattering by electrons at a constant electron density. In the case of scattering by electrons we obtain from (7) and (14)

$$\frac{\Delta E_{\perp}}{\Delta x} = \frac{m}{2M} \frac{dE}{dx}. \tag{24}$$

From this we get in accordance with (8)

$$\frac{1}{2} \left\langle \frac{\Delta E_{\perp}^2}{\Delta x} \right\rangle = \frac{m}{2M} \frac{dE}{dx} \langle (E_{\perp} - U(r)) \rangle. \tag{25}$$

The expression  $\langle E_{\perp} - U(r) \rangle$  is obviously the average kinetic energy. If the potential is approximated by a square well, then  $\langle E_{\perp} - U(r) \rangle \approx E_{\perp}$ .

In the calculation of  $(\Delta E_{\perp} / \Delta x)_e$  in the free-electron model, it should be borne in mind that only short-range collisions contribute to  $\Delta E_{\perp}$ . Without taking into account the contribution of the internal electrons to  $\Delta E_{\perp}$ , we have here

$$\left( \frac{\Delta E_{\perp}}{\Delta x} \right)_e = \frac{m}{M} \frac{4\pi Z_1 e^4 \rho_V}{mv^2} \ln \left| \frac{2m\nu v_F}{\hbar\omega_p} \right|,$$

where  $\hbar\omega_p$  is the plasmon energy,  $\rho_V = NZ_V$ ,  $Z_V$  is the number of valence electrons participating in the plasma oscillations, and  $v_F$  is the Fermi velocity.

Substituting (25) in (13), we obtain the diffusion equation

$$\frac{\partial f}{\partial x} = \frac{m}{2M} \frac{dE}{dx} \frac{\partial}{\partial E_{\perp}} E_{\perp} \frac{\partial f}{\partial E_{\perp}}, \tag{26}$$

or in terms of the momentum defined by  $p_{\perp}^2 / 2M = E_{\perp}$ ,

$$\frac{\partial f}{\partial x} = \frac{m}{4} \frac{dE}{dx} \frac{\partial}{\partial p_{\perp}} \left( p_{\perp} \frac{\partial f}{\partial p_{\perp}} \right). \tag{27}$$

Finally, changing over from the particle coordinates to the particle energy with the aid of the relation

$$x = \int_E^{E_0} \left( \frac{dE}{dx} \right)^{-1} dE,$$

we obtain

$$\frac{\partial f}{\partial E} = \frac{m}{4} \frac{\partial}{\partial p_{\perp}} \left( p_{\perp} \frac{\partial f}{\partial p_{\perp}} \right). \tag{28}$$

We seek a solution of this equation by separating the variables under the boundary condition  $F(E, E_{cr}) = 0$ , where  $E_{cr}$  is Lindhard's critical transverse energy. This condition means that we neglect completely the flux of channeled ions per unit solid angle for angles close to the critical Lindhard angle, assuming it to be much smaller than the corresponding density for the channeled particles. Such an abrupt boundary is observed experimentally in the registration of the angular distribution of a beam passing through a thick crystal along the crystallographic axis. We then obtain the following solution:

$$f = \sum_{n=1}^{\infty} a_n \exp \left\{ -\frac{\mu_n^2 m}{8M} \frac{E_0 - E}{E_{\perp cr}} \right\} J_0 \left( \frac{p_{\perp}}{p_{\perp cr}} \mu_n \right), \tag{29}$$

where  $J_0$  is a Bessel function,  $\mu_n$  is its  $n$ -th zero,  $p_{\perp cr} = \sqrt{2ME_{\perp cr}}$ , and

$$a_n = \frac{2}{p_{\perp cr}^2 J_1^2(\mu_n)} \int_0^{p_{\perp cr}} f(E_0, E_{\perp}) J_0 \left( \mu_n \frac{p_{\perp}}{p_{\perp cr}} \right) p_{\perp} dp_{\perp}. \tag{30}$$

For normal incidence of the ion beam on the crystal we have  $f(E_0, E_{\perp}) = \delta(E_{\perp})$  if the particle flux trapped in the channel is normalized to unity. Then

$$a_n = 2M / p_{\perp cr}^2 J_1^2(\mu_n). \tag{31}$$

At  $m(E_0 - E) / 8ME_{\perp cr} \geq 1$  we can obviously confine ourselves to several harmonics in the expansion (29).

The ion flux in the channel is

$$I = \int_0^{E_{\perp cr}} f dE_{\perp} = \sum_{n=1}^{\infty} \frac{a_n p_{\perp cr} J_1(\mu_n)}{M \mu_n} \exp \left\{ -\frac{\mu_n^2 m}{8} \frac{E_0 - E}{E_{\perp cr}} \right\}, \tag{32}$$

or, after substituting (31),

$$I = \sum_{n=1}^{\infty} \frac{2}{\mu_n J_1(\mu_n)} \exp \left\{ -\frac{\mu_n^2 m}{8} \frac{E_0 - E}{E_{\perp cr}} \right\}. \tag{32'}$$

#### 4. COMPARISON WITH EXPERIMENT AND DISCUSSION OF RESULTS

Let us consider the dechanneling of protons with  $E = 3$  MeV in tungsten in the Thomas-Fermi model. This case was investigated experimentally by Foti et al.<sup>[9]</sup> In the Thomas-Fermi model, the electron density decreases rapidly with increasing distance from the atomic chain. The distribution of the lattice vibrations with respect to the amplitudes of the thermal vibrations can be regarded as Gaussian, with an rms displacement  $\rho_{\perp}$  which is much smaller than the channel dimensions. In this case the ion scattering occurs mainly at the shortest approach of the ions to the atomic chain, when the angle is  $\theta \approx 0$ . This entails a monotonic increase of  $E_{\perp}$ , so that the spreading of the ions with respect to  $E_{\perp}$  can be neglected. Such an approximation was proposed by Lindhard<sup>[3]</sup> and was used by a number of authors<sup>[9,12]</sup>; it can apparently be used for estimates. To simplify the calculations we assume that the average ion energy loss in the channel  $(dE/dx)_k$  is proportional to the loss in amorphous matter  $(dE/dx)_n$ <sup>[8]</sup>

$$(dE/dx)_k = \lambda (dE/dx)_n. \tag{33}$$

In tungsten we have  $\lambda = 0.44$  at  $E \approx 3$  MeV. For fast particles  $dE/dx$  is proportional to  $1/E$ , and consequently  $E = E_0(1 - 2x/L)^{1/2}$ , where  $L = m(\lambda B M \psi_1^2)^{-1}$ ,  $B$  and  $\psi_1$  are taken at  $E = E_0$ ,  $L = 25 \mu$  at  $\lambda = 1$  and  $\alpha = 3.14 \text{ \AA}$ .

From (15) and (18) we obtain the connection between the range to dechanneling and the initial transverse energy  $\epsilon_{\perp}$ :

$$\int_{\epsilon_{\perp}}^2 \left( \frac{\Delta \epsilon_{\perp}}{\Delta x} \right)_{\epsilon=E_0}^{-1} d\epsilon_{\perp} = \int_0^x \left( 1 - \frac{2x}{L} \right)^{-1/2} dx \tag{34}$$

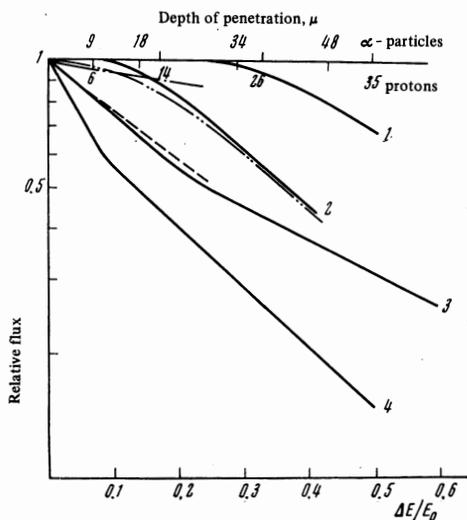
or

$$L \left[ 1 - \left( 1 - \frac{2x}{L} \right)^{1/2} \right] = \frac{A}{\kappa B} \int_{\epsilon_{\perp}}^{\epsilon_{\perp}^0} \frac{d\epsilon_{\perp}}{1 - \epsilon_{\perp}/A} \times \left[ \frac{2t^3}{3A^2} + t^2 \left( \frac{2}{3A^2} - \frac{1}{A} \right) + t \left( \frac{2}{3A^2} - \frac{1}{A} - 1 + \frac{1}{\kappa} \right) + A^2 \right]^{-1}. \tag{35}$$

The denominator of the integrand has four roots:  $t_0 = A$ ,  $t_1 = -1.39$ , and  $t_{2,3} = 0.963 \pm i0.394$  for channeling in the  $\langle 100 \rangle$  direction at a temperature  $25^{\circ}\text{C}$ . The fraction of particles having an initial transverse energy larger than  $\epsilon_{\perp}$  is obviously

$$\chi = \frac{r_1^2}{r_0^2} = \frac{A - 1}{A \exp \epsilon_{\perp} - 1}. \tag{36}$$

The dependence of the fraction of the dechanneled particles on the depth of penetration is obtained by calculating the integral (35) and substituting the  $\epsilon_{\perp}(\chi)$  relation determined by formula (36). The pole  $t_1 = -1.39$  makes a very small contribution, since it is



Dependence of the relative flux of channeled ions on the depth of penetration into the crystal (or on the relative energy loss  $\Delta E/E_0$ ). Curves 1, 2—square-well approximation of the potential for protons penetrating in the  $\langle 100 \rangle$  direction at 3 MeV into W and for  $\alpha$  particles penetrating into Si in the  $\langle 110 \rangle$  direction at 7 MeV, respectively; curves 3 and 4—the same for the oscillator-potential model; dash-dot curve—approximation of monotonic increase of transverse energy for protons in W at 3 MeV (absence of diffusion); dashed curve—results of experiment on backward scattering; dash with two dots—results of transmission experiment.

located far from the integration region. The poles  $t_{2,3}$  do not occur if scattering by thermal vibrations is not included. Their influence, however, is appreciable, since  $x$  depends nonlinearly on  $\delta\epsilon_{\perp}$  and a strong interference occurs between the electronic contribution and the contribution due to thermal vibrations. The principal pole is  $t_0 = A$ , which remains also when the scattering is only by electrons. The depth  $x_{1/2}$  at which half the ions leave the channel is then equal to 28 and 38  $\mu$ , if we disregard the thermal vibrations. The dependence of the depth on the fraction of the dechanneled ions at  $\chi \gtrsim 0.1$  turns out to be

$$L[1 - (1 - 2x/L)^{1/2}] \approx 15 \{ \ln [1 + \chi(A - 1)] - 0.3 \}$$

or

$$\chi \approx \frac{1}{44} \{ 1.3 \exp [L(1 - (1 - 2x/L)^{1/2})] - 1 \}.$$

From this we obtain a much smaller value of  $\chi$  than obtained by Foti et al.<sup>[9]</sup> (see the figure). This is caused by the fact that  $3a^2/r_0^2 = 1/44$ , and  $1/15$  as given in<sup>[9]</sup>. This result indicates that in the present case the principal term is the electronic rather than nuclear scattering. It is, however, too sensitive to the value of the potential at the center of the channel. The reason for this is that the density at the center of the channel is chosen to be very low in the single-chain approximation, and since most particles begin to acquire transverse energy  $\epsilon_{\perp}$  with small values of  $\epsilon_{\perp}$ , this results in larger depths of dechanneling.

The diffusion approximation considered in Sec. 3 is free of this shortcoming, since it is less sensitive to the details of the electron distribution. This approximation should therefore give better results at  $\chi \sim 0.1$ —0.5 than the approximation in which the transverse energy increases continuously. The result of the calculation by means of formula (32') is shown in the figure.

To ascertain the influence of the potential, we also performed calculations with a harmonic potential. In this case the solution of (13') for normal incidence of the beam on the crystal is

$$f_0 = \sum_{n=1}^{\infty} \frac{2(1 - J_0(\mu_n))}{\mu_n J_0^2(\mu_n)} \exp \left\{ -\frac{\mu_n^2}{16} \frac{m}{M} \frac{E_0 - E}{E_{Lcr}} \right\} \times J_1 \left[ \mu_n \left( \frac{\epsilon_{\perp}}{\epsilon_{Lcr}} \right)^{1/2} \right] \frac{\epsilon_{\perp}^{1/2}}{\epsilon_{Lcr}^{1/2}},$$

where  $f_0$  is the number of particles in the channel, normalized to unity,  $\mu_n$  is the zero of the function  $J_1$ , and

$$\int_0^{\epsilon_{Lcr}} f_0 d\epsilon_{\perp} = 1.$$

The fraction of the dechanneled particles is in this case

$$\chi = \sum_{n=1}^{\infty} \left( \frac{2}{\mu_n} \right)^2 [1 - J_0^{-1}(\mu_n)] \left[ 1 - \exp \left\{ -\frac{\mu_n^2}{16} \frac{m}{M} \frac{E_0 - E}{E_{Lcr}} \right\} \right].$$

The figure shows the results of the calculation by this formula for protons and  $\alpha$  particles in tungsten and in silicon.

The dechanneling of  $\alpha$  particles passing through single crystals of silicon was investigated by Bulgakov and the authors<sup>[10]</sup>. The depth  $x_{1/2}$  obtained in this case was 40  $\mu$ . It is seen from the figure that the value of  $x_{1/2}$  obtained theoretically by solving the diffusion equation in which only electron scattering is taken into account is 44  $\mu$  in the square-well potential approximation. We also calculated  $x_{1/2}$  for this case in the approximation wherein  $E_{\perp}$  increases continuously in accordance with formula (35). This yielded for  $x_{1/2}$  the values 43  $\mu$  in scattering by electrons and 32  $\mu$  when scattering by thermal vibrations is added. In this case the agreement with experiment is better than for protons in tungsten, and the value of the main contribution of the electrons to the dechanneling is also confirmed.

In the present study we obtained the Fokker-Planck equation with allowance for the diffusion of the particles with respect to the transverse energy. The previously employed approach<sup>[9,11,12]</sup> is approximate when compared with ours, since no account was taken of the diffusion<sup>[9,11]</sup> or of the inhomogeneity of the particle flux in the channel<sup>[12]</sup>.

The calculations show that the classical theory of multiple scattering, based on the solution of the Fokker-Planck equation, gives satisfactory agreement with experiment. In many cases, for example when ions pass through silicon and tungsten, the scattering by electrons is the dominant factor leading to the dechanneling. This makes it possible to neglect the contribution of the thermal vibrations to multiple scattering and to solve the diffusion approximation analytically with sufficient accuracy.

In conclusion, the authors are sincerely grateful to O. B. Firsov for constant interest in the work and for a useful discussion.

## APPENDIX

The Fokker-Planck equation for the distribution function  $f(p, r, t)$  is

$$\frac{\partial f}{\partial t} + \mathbf{p} \nabla f - \nabla U \text{grad}_p f + \text{div } \mathbf{I} = 0,$$

where  $\mathbf{I}$  is the flux due to the collisions. According to Landau<sup>[13]</sup>, in Coulomb interaction, this flux is equal to

$$I_p = \frac{\Delta p}{\Delta t} f, \quad I_\theta = -\frac{1}{4} \frac{\Delta p_\perp^2}{\Delta t} \frac{\partial f}{p \partial \theta}$$

(we have used here a spherical coordinate system;  $\theta$  is the angle between  $\mathbf{p}$  and the chosen polar axis, which in our case is the  $x$  axis of the channel; in addition, azimuthal symmetry is assumed).

Let us calculate  $\text{div } \mathbf{I}$  integrated over the entire accessible region. It is convenient here to change over to the variables  $p_x$  and  $E_\perp$ . We have

$$\text{div } \mathbf{I} = \frac{1}{p^2} \frac{\partial}{\partial p} p^2 \frac{\Delta p}{\Delta t} f - \frac{1}{4} \frac{1}{p^2 \sin \theta} \frac{\partial}{\partial p} \sin \theta \frac{\Delta p_\perp^2}{\Delta t} \frac{\partial f}{\partial \theta}.$$

We make the substitution

$$p, \theta \rightarrow p_x, E_\perp; \quad p_x^2 \approx p^2(1 - \theta^2/2) \approx p^2; \\ E_\perp \approx p^2 \theta^2 / 2M + U(r).$$

We obtain

$$\text{div } \mathbf{I} = \frac{1}{p_x^2} \frac{\partial}{\partial p_x} \left( p_x^2 \frac{\Delta p}{\Delta t} f \right) + \frac{\theta^2}{M} \frac{\partial}{\partial E_\perp} p_x \frac{\Delta p}{\Delta t} f \\ - \frac{1}{2} M \frac{\partial}{\partial E_\perp} \left( [E_\perp - U(r)] \frac{\Delta p_\perp^2}{\Delta t} \frac{\partial f}{\partial E_\perp} \right).$$

We have retained here the second term  $\sim \theta^2$ , for when ions are scattered by electrons the value of  $\Delta p_\perp^2 / \Delta t$  is smaller by a factor  $m/M$  than  $p_x \Delta p / \Delta t$ . We shall no longer distinguish between  $p$  and  $p_x$ :

$$\text{div } \mathbf{I} = \frac{1}{p^2} \frac{\partial}{\partial p} \left( p^2 \frac{\Delta p}{\Delta t} f \right) + \frac{2(E_\perp - U(r))}{p} \frac{\partial}{\partial E_\perp} \left( \frac{\Delta p}{\Delta t} f \right) \\ - \frac{1}{2} \frac{\partial}{\partial E_\perp} \left( [E_\perp - U(r)] \frac{\Delta p_\perp^2}{M \Delta t} \frac{\partial f}{\partial E_\perp} \right).$$

The distribution function  $f(p, E_\perp, \mathbf{r}, t)$ , after statistical equilibrium is attained in the accessible region, corresponds to the microcanonical ensemble

$$f(p, E_\perp, \mathbf{r}, t) = \begin{cases} F(p, E_\perp, t) & \text{for } E_\perp \geq U(r), \\ 0 & \text{for } E_\perp < U(r). \end{cases}$$

$F(p, E_\perp, t) dE_\perp dp$  is the number of particles per unit volume in the interval  $dE_\perp dp$ . Integration of  $\text{div } \mathbf{I}$  leads to the following expression:

$$\int \text{div } \mathbf{I} 2\pi r dr = \frac{1}{p^2} \frac{\partial}{\partial p} \left\{ \left[ p^2 \int_{r_1}^{r_0} \frac{\Delta p}{\Delta t} 2\pi r dr \right] F \right\} \\ + \frac{2}{p} \left\{ \int_{r_1}^{r_0} \frac{\Delta p}{\Delta t} (E_\perp - U(r)) 2\pi r dr \right\} \frac{\partial F}{\partial E_\perp} - \frac{\partial}{\partial E_\perp} \\ \times \left\{ \left[ \int_{r_1}^{r_0} (E_\perp - U(r)) \frac{\Delta p_\perp^2}{2M \Delta t} 2\pi r dr \right] \frac{\partial F}{\partial E_\perp} \right\},$$

where  $r_1$  is determined from the condition  $E_\perp = U(r_1)$ . Let us write down the particle energy balance equation<sup>[1]</sup>:

$$\pi(r_0^2 - r_1^2) \frac{\partial F}{\partial t} + \int \text{div } \mathbf{I} 2\pi r dr = 0.$$

From this we obtain ultimately

<sup>1</sup>A similar method was used by Tverskoĭ<sup>[14]</sup> in the problem of particle scattering in a geomagnetic trap.

$$\frac{\partial F}{\partial t} = \frac{1}{S(E_\perp)} \frac{\partial}{\partial E_\perp} S(E_\perp) \left\langle (E_\perp - U) \frac{\Delta E_\perp}{\Delta t} \right\rangle \frac{\partial F}{\partial E_\perp} \\ - \frac{1}{E} \left\langle (E_\perp - U) \frac{\Delta E}{\Delta t} \right\rangle \frac{\partial F}{\partial E_\perp} - \frac{1}{p^2} \frac{\partial}{\partial p} p^2 \left\langle \frac{\Delta p}{\Delta t} \right\rangle F,$$

where the averaging denotes

$$\langle x \rangle = \frac{1}{S(E_\perp)} \int_{r_1}^{r_0} x 2\pi r dr,$$

and  $\Delta E_\perp = \Delta p_\perp^2 / 2M$  is the increment of the transverse energy;  $S(E_\perp) = \pi(r_0^2 - r_1^2)$ . The fluctuation term is

$$\left\langle \left( \frac{1}{2} \frac{\Delta E_\perp^2}{\Delta t} \right) \right\rangle = \left\langle \frac{\Delta E_\perp}{\Delta t} (E_\perp - U(r)) \right\rangle.$$

Hence

$$\left\langle \frac{\Delta E_\perp}{\Delta t} \right\rangle = \frac{1}{2} \frac{\partial}{\partial E_\perp} \left\langle \frac{\Delta E_\perp^2}{\Delta t} \right\rangle,$$

if  $S$  does not depend on  $E_\perp$ . Thus, without account of deceleration and when  $S(E_\perp) = \text{const}$  (at  $r_0 \gg r_1$ ), the Fokker-Planck equation goes over into a diffusion equation in the form

$$\partial F / \partial t = \text{div } D \text{grad } F.$$

The obtained Fokker-Planck equation can be transformed after changing over to the distribution function  $f(E, E_\perp, t)$  in accordance with the relation

$$F(p, E_\perp, t) dE_\perp dp = f(E, E_\perp, t) dE_\perp dE$$

to the traditional form

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial E_\perp} \left[ \left\langle \frac{\Delta E_\perp}{\Delta t} (E_\perp - U(r)) \right\rangle \frac{\partial f}{\partial E_\perp} \right] - \frac{\partial}{\partial E} \\ \times \left[ \left( \left\langle \frac{\Delta E_\perp}{\Delta t} \right\rangle + \left\langle \frac{\Delta E_\perp}{\Delta t} \right\rangle_{\text{dec}} \right) f \right] - \frac{\partial}{\partial E} \left[ \left\langle \frac{\Delta E}{\Delta t} \right\rangle f \right]$$

where

$$\left\langle \frac{\Delta E_\perp}{\Delta t} \right\rangle_{\text{dec}} = \frac{1}{E} \left\langle \frac{\Delta E}{\Delta t} (E_\perp - U(r)) \right\rangle.$$

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