

Statistical theory of charge state distributions of channeled heavy ions

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(Received 22 March 2005; revised manuscript received 11 July 2005; published 14 September 2005)

On the basis of the kinetic equations, a theory of transmission of multiply charged heavy ions through crystals is developed. It takes into account both diffusion in transverse momentum and charge exchange. The theory gives an adequate description of observed angular distributions of heavy ions transmitted through a crystal, allows calculation of the partial angular distributions of the various charge states, and gives a physical explanation of the so called cooling maxima and the heating minima in the angular distributions. The occurrence of cooling or heating effects and the detailed structure of the angular distribution depend on both the impact parameter dependence of the probabilities for electron capture and loss and on the relative contributions from different charge states. Since the angular distributions can be very different for different charge states, the structure of the total distribution can be quite complex.

DOI: [10.1103/PhysRevB.72.094109](https://doi.org/10.1103/PhysRevB.72.094109)

PACS number(s): 61.85.+p, 34.70.+e, 34.20.Cf, 34.10.+x

I. INTRODUCTION

When heavy ions pass through crystals, the ion-atom collisions cause fluctuations of the heavy ion charge due to the loss or capture of electrons. The interest in such changes of the charge state is based on the fact that the obtained data can provide important information about the character of the atomic collisions. For the first time, this phenomenon was studied in Ref. 1, and it has been under active investigation until now. Since that time, there have been many studies dedicated to the measurement of the charge state distribution and the determination of the average equilibrium charge state of the heavy ions. A detailed review of this subject can be found in Refs. 2–4.

In the present work, we are interested in another, less explored, problem, namely the study of new phenomena that appear when heavy ions pass through a crystal along a major crystallographic direction. Recently,^{5–9} it has been shown that the penetration of heavy ions through crystals is accompanied by a breaking of the isotropy of the angular distributions of an originally isotropic ion beam.

The systematic experimental research for various crystals has shown the existence of so-called “cooling or “heating” of ion transmitted through the crystal along a major crystallographic direction.¹⁰ These effects depend not only on the type of a target, but also on the energy of ions.

The effects violate a basic principle in the physics of channeling phenomena,¹¹ the so-called principle of detailed balance (or reciprocity). This means that the kinetics of the penetration of the heavy ions in crystals is essentially not in equilibrium. The attention to this problem has been drawn by Ref. 5. A hypothesis of a significant influence of charge exchange on the dynamics and the kinetics of ions transmitted through oriented crystals was stated there.

A theoretical investigation of the evolution of charge states for channeled heavy ions is motivated by the need to calculate the probabilities of the charge changing processes to describe the interaction of ions with nuclear chains and planes.¹² Essential progress can be achieved with the help of computer simulations.^{13,14} A description of the phenomenon has been undertaken in Ref. 10 by means of the n -body clas-

sical transport Monte Carlo method, which lead to encouraging results. However, Monte Carlo calculations are very time consuming and not as accurate as the description via the kinetic channeling theory.¹⁵

Compared to usual channeling calculations,¹⁶ the statistical description of the charge exchange effects is complicated by the introduction of an additional dimension, a new discrete variable Q indicating the charge state. In this case the kinetics of ions in an oriented crystal is described by a set of kinetic equations whose number is equal to the ion atomic number Z_1 . This approach enables one to study the evolution of the charge states with depth for channeled and quasichanneled (or “under-barrier” and “above-barrier”) ions when they propagate through the crystal. This is essentially different from the movement through amorphous materials. The evolution with depth of the charge state distribution leads to a redistribution of the flux of ions in the crystal and, finally, changes the character of their interaction with the crystal. This allows one, not only to explain the variety of observed effects, but also to obtain fundamental data on the interaction of multicharged heavy ions with crystals.

There are three basic assumptions in the kinetic channeling theory of heavy ions with charge exchange effects.

First, the model is based on the continuum theory of channeling.^{11,15–17} Also, in the kinetic equations we have neglected the change of the longitudinal component of an ion momentum directed along a crystallographic direction. Such an approach is applicable for not too thick targets and is successfully used in studies of structural features of crystals by a channeling technique.^{18,19}

Second, it is supposed that the initial condition of an ions beam is a noncoherent ensemble homogeneously filling the accessible area in a transverse plane normal to the crystallographic direction. In this case all impact parameters are equiprobable, which allows averaging the probability of ion interaction with a crystal over the accessible area. The accessible area is defined as area in the transverse plane, occupied by the particles with fixed transverse energy.

Third, the duration of electron loss and capture processes and the duration of multiple scattering or the excitation of electron-phonon subsystem of crystal are very different. The

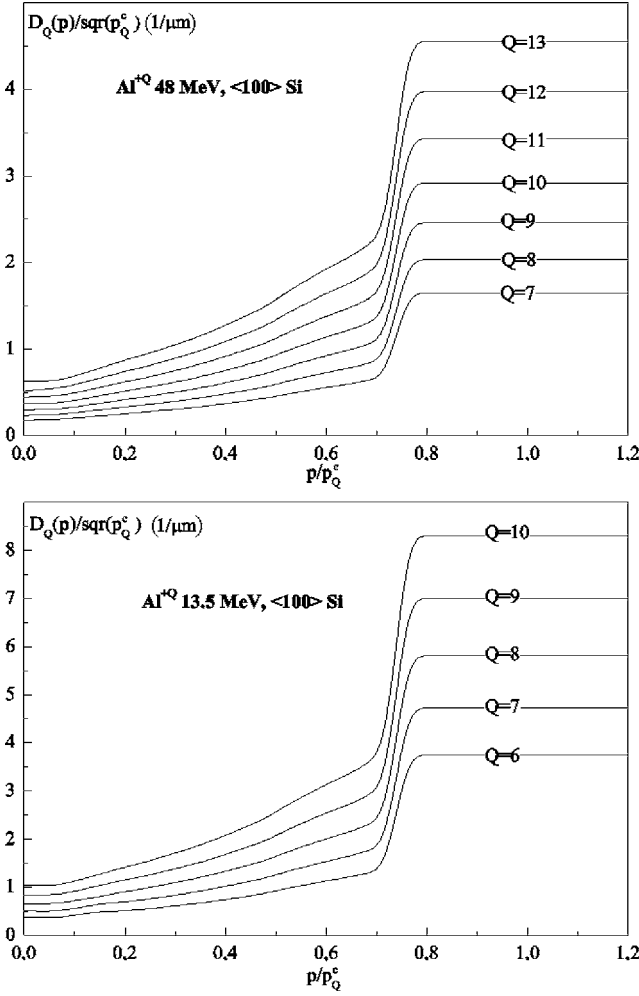


FIG. 1. Diffusion coefficients of Al^{+Q} ions in the $\langle 100 \rangle$ channel of a Si crystal.

first processes are fast and their characteristic time is much less than the second one.¹³ This allows one to factorize the probability of the combined process containing the electron loss or capture and to write it down as a product of probabilities of separate processes.

II. BASIC EQUATION

The assumptions specified above correspond to a statistical equilibrium in the transverse phase space, which leads to the uniform distribution over the coordinates and azimuthal angles inside the accessible area for ions. Usually the basic kinetic equation for channeling is expressed in terms of the transverse energies, as it has been done in Refs. 15–17. Here we use the representation of the kinetic equation in terms of transverse momentums.

The state of a particle in the channel with the fixed transverse energy is defined by a phase trajectory in four-dimensional space of transverse momentum and coordinates $\{\mathbf{p}, \mathbf{r}\}$. Phase trajectories in an axial case are not closed because the potential in the axial channel is not harmonious. Therefore the phase trajectory fills in densely some volume in space $\{\mathbf{p}, \mathbf{r}\}$, which is defined by the value of transverse

TABLE I. The adjusting values of α , Q_0 , r_c , and r_l for an Al^{+Q} ion at the different projectile energy.

Energy, MeV	Q_0	α	r_c , Å	r_l , Å
13.5	8	0.8	0.38	0.17
48 (Ref. 13)	10	0.5	0.20	0.30

energy (the sum of potential and kinetic energy). The projection of this volume to the spatial axes $\{\mathbf{r}\}$ defines so-called accessible area.

For the positively charged particles (in contrast with the negative ones) the continuous potential is nearly zero in the wide range of transverse coordinates. The axially channeled positively charged particles spend the greatest time in this part of the channel where continuous potential is approximately constant in the wide range. So we can consider the distribution function dependent only on transverse momentum and depth of penetration of particles in a crystal. Such an approach was used by Lindhard in Ref. 11 as one of approximation in which the potential in a transverse plane have been estimated by a rectangular well. In this case the kinetic equation for distribution function looked like diffusion Fick equation in transverse momentum space (see also Ref. 21).

So the two-dimensional \mathbf{p} vector is really the square root of the transverse energy and that its direction does not have a physical meaning. Otherwise the \mathbf{p} vector is the momentum at large distances from the atomic rows, but the direction of the vector is not defined because it changes rapidly due to collisions with the rows. So the transverse accessible area of the ion can be expressed approximately as a function of the modulus of the transverse momentum.

Such the approximation simplifies the treatment and is not a bad for positively charged particles in axial channeling. This approach takes into account the flux redistribution too [e.g., see Eq. (2) and Fig. 3 in Ref. 18] and has been successfully used in the channeling calculations in Refs. 18–20. Such a representation seems to be excessive, as it demands an additional degree of freedom in an axial case. However, it allows obtaining the transmission angular distributions directly and by and large enables us to study the processes with the violated azimuthal symmetry.

The evolution of the distribution $f_Q(\mathbf{p}, z)$ with depth z in transverse momentum can be described by the Smolukhovsky equations:

$$\frac{\partial f_Q(\mathbf{p}, z)}{\partial z} = \sum_{Q'} \int d^2q [w_{Q'Q}(\mathbf{p} + \mathbf{q}, \mathbf{q}) f_{Q'}(\mathbf{p} + \mathbf{q}, z) - w_{QQ'}(\mathbf{p}, \mathbf{q}) f_Q(\mathbf{p}, z)]. \quad (1)$$

Let us define the transition probability per unit of depth with change of the charge state $Q \rightarrow Q'$ and transverse momentum $\mathbf{p} \rightarrow \mathbf{p}' = \mathbf{p} - \mathbf{q}$ in the position $\mathbf{r} = (x, y)$ of the transverse plane as $w_{Q'Q}(\mathbf{r}, \mathbf{p}, \mathbf{q}) d^2q$. Under the assumptions specified above, the transition probability $w_{Q'Q}(\mathbf{p}, \mathbf{q}) d^2q$ averaged over the accessible area is equal to

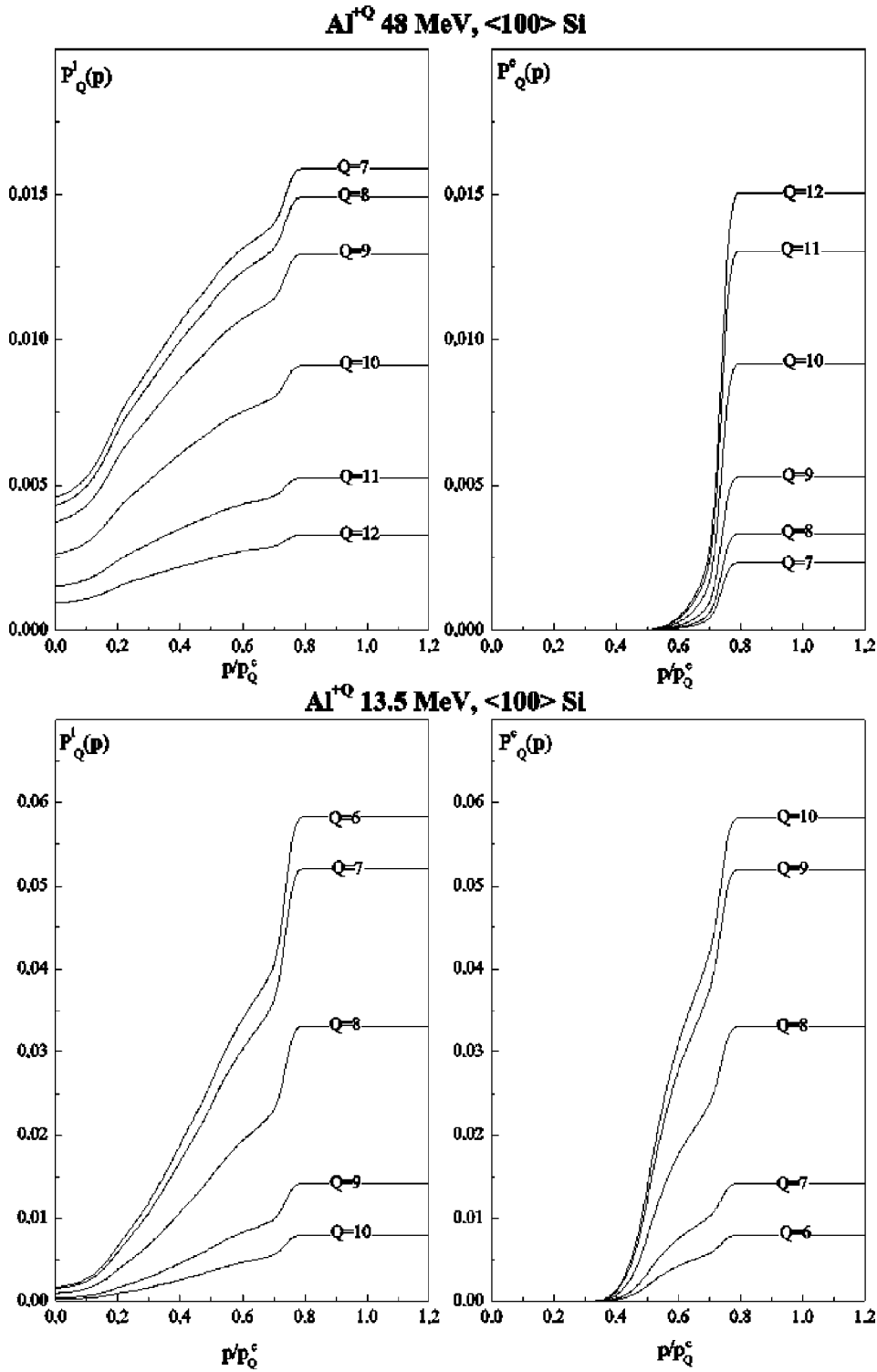


FIG. 2. Electron capture and loss probabilities for Al^{+Q} ions in the $\langle 100 \rangle$ channel of a Si crystal.

$$w_{QQ'}(\mathbf{p}, \mathbf{q}) = \frac{1}{S_Q(\mathbf{p})} \int_{S_Q(\mathbf{p})} w_{QQ'}(\mathbf{r}, \mathbf{p}, \mathbf{q}) d^2r. \quad (2)$$

The value of the accessible area $S_Q(\mathbf{p})$ in the transverse plane and the integration regions in (2) is determined by the equation

$$\frac{\mathbf{p}^2}{2M_1} \geq U_Q(\mathbf{r}) - U_Q^{(\min)}, \quad (3)$$

where $U_Q(\mathbf{r})$ is the continuum potential in the transverse plane for a charge Q , $U_Q^{(\min)}$ is the minimum value of the potential, and M_1 is the mass of incident ions.

Usually the function $w_{QQ'}(\mathbf{p}, \mathbf{q})$ quickly decreases with an increase of transverse momentum transferred to the crystal. So, the small values of \mathbf{q} play the basic role in the integral

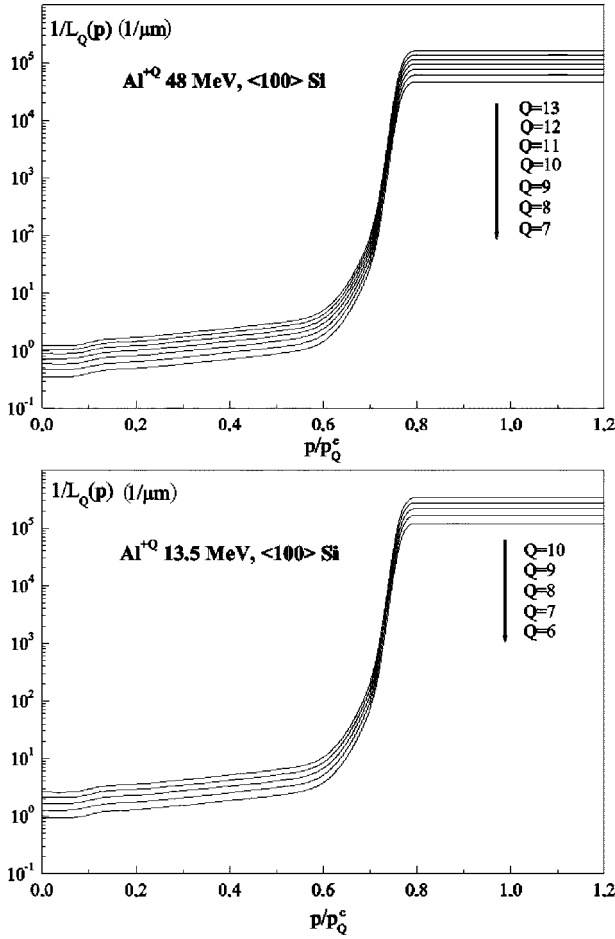


FIG. 3. Length of the free path of Al^{+Q} ions in the $\langle 100 \rangle$ channel of a Si crystal.

(1). This allows one to expand the integrand in a Taylor series. Neglecting terms above the second order, the kinetic equations can be written in the form

$$\frac{\partial f_Q(\mathbf{p}, z)}{\partial z} = \sum_{Q'} \left[W_{Q'Q}(\mathbf{p}) f_{Q'}(\mathbf{p}, z) - W_{QQ'}(\mathbf{p}) f_Q(\mathbf{p}, z) + \frac{\partial}{\partial p_\alpha} \left(A_{Q'Q}^\alpha f_{Q'}(\mathbf{p}, z) + D_{Q'Q}^{\alpha\beta} \frac{\partial}{\partial p_\beta} f_{Q'}(\mathbf{p}, z) \right) \right], \quad (4)$$

where the charge exchange probability $W_{Q'Q}(\mathbf{p})$, the “generalized” diffusion coefficients $D_{Q'Q}^{\alpha\beta}$, and the dynamic friction $A_{Q'Q}^\alpha$ are given by ($\alpha, \beta = 1, 2$)

$$W_{Q'Q}(\mathbf{p}) = \int w_{Q'Q}(\mathbf{p}, \mathbf{q}) d^2 q, \quad (5)$$

$$D_{Q'Q}^{\alpha\beta} = \frac{1}{2} \int q_\alpha q_\beta w_{Q'Q}(\mathbf{p}, \mathbf{q}) d^2 q, \quad (6)$$

$$A_{Q'Q}^\alpha = \int q_\alpha w_{Q'Q}(\mathbf{p}, \mathbf{q}) d^2 q + \frac{\partial}{\partial p_\beta} D_{Q'Q}^{\alpha\beta}.$$

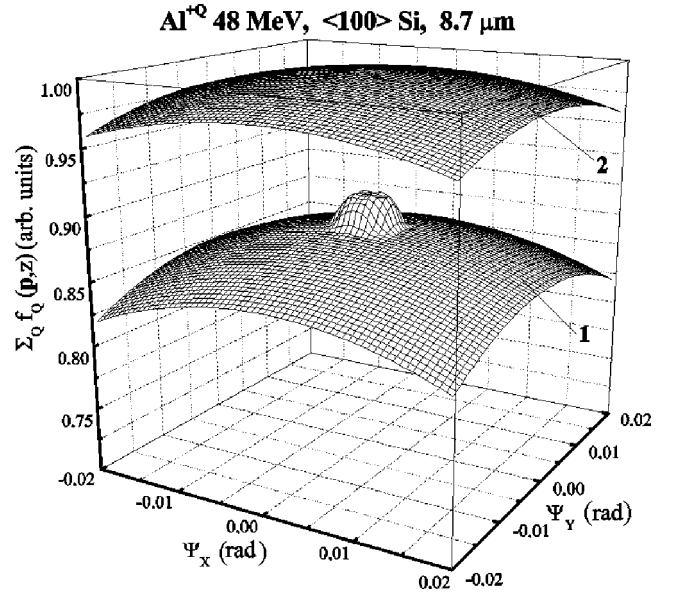


FIG. 4. Calculated axial angular 3D distribution of Al^{+Q} ions after transmission of an $8.7 \mu\text{m}$ Si $\langle 100 \rangle$ crystal (1). Surface (2) illustrates the calculated angular 3D distribution, in accordance with Eq. (12), in which $P_Q^{c,l}(\mathbf{p}) = 0$.

It is convenient to write down the probability $w_{QQ'}(\mathbf{p}, \mathbf{q})$ as the sum of two terms. We can then distinguish between the processes occurring without change and with a change of the charge state, respectively,

$$w_{QQ'}(\mathbf{p}, \mathbf{q}) = \delta_{QQ'} w_Q^{(1)}(\mathbf{p}, \mathbf{q}) + (1 - \delta_{QQ'}) w_{QQ'}^{(2)}(\mathbf{p}, \mathbf{q}), \quad (7)$$

where $\delta_{QQ'} = 1$ if $Q = Q'$; and $\delta_{QQ'} = 0$ if $Q \neq Q'$.

A theoretical analysis of the kinetic equations (4) is very difficult. In particular, because one needs to calculate in advance the kinetics coefficients on the basis of the microscopic theory. Then Eq. (4) simplifies significantly if we assume that the charge exchange is dominated by processes with unit charge change, that is, $Q' \rightarrow Q \pm 1$.

The processes of electron capture and loss are fast processes that occur over depths of several hundred Å. This is much less than characteristic length of multiple scattering of ions in a crystal, which is several thousand Å. In this case, the probability $w_{QQ'}^{(2)}(\mathbf{p}, \mathbf{q})$ in Eq. (7) can be written in the factorized form of separate processes. So, for the single-electron exchange processes,

$$w_{Q,Q+1}^{(2)}(\mathbf{p}, \mathbf{q}) = P_Q^l(\mathbf{p}) w_{Q+1}^{(1)}(\mathbf{p}, \mathbf{q}),$$

$$w_{Q,Q-1}^{(2)}(\mathbf{p}, \mathbf{q}) = P_Q^c(\mathbf{p}) w_{Q-1}^{(1)}(\mathbf{p}, \mathbf{q}), \quad (8)$$

$$P_Q^{c,l}(\mathbf{p}) = \frac{1}{S_Q(\mathbf{p})} \int_{S_Q(\mathbf{p})} P_Q^{c,l}(\mathbf{r}) d^2 r, \quad (9)$$

where $P_Q^c(\mathbf{r})$ and $P_Q^l(\mathbf{r})$ are the probabilities of electron capture and loss of ion in charge state Q , respectively; of course, $P_Q^c(\mathbf{r})$ and $P_Q^l(\mathbf{r})$ depend on the impact parameter. The charge exchange probability $W_{Q'Q}(\mathbf{p})$ in this approach can be written as

$$W_{Q,Q+1}(\mathbf{p}) = \frac{1}{L_{Q+1}(\mathbf{p})} P_{Q+1}^l(\mathbf{p}), \quad W_{Q,Q-1}(\mathbf{p}) = \frac{1}{L_{Q-1}(\mathbf{p})} P_{Q-1}^c(\mathbf{p}), \quad (10)$$

$$W_{Q-1,Q}(\mathbf{p}) = \frac{1}{L_Q(\mathbf{p})} P_{Q-1}^l(\mathbf{p}), \quad W_{Q+1,Q}(\mathbf{p}) = \frac{1}{L_Q(\mathbf{p})} P_{Q+1}^c(\mathbf{p}), \quad (11)$$

where

$$1/L_Q(\mathbf{p}) = \int w_Q^{(1)}(\mathbf{p}, \mathbf{q}) d^2q.$$

It is worth noting that it is possible to define $L_Q(\mathbf{p})$ as a length of free path of ion with a transverse momentum \mathbf{p} and charge state Q .

We shall suppose in what follows that the probability $w_{QQ'}(\mathbf{r}, \mathbf{p}, \mathbf{q}) d^2q$ depends on the modulus of the transferred momentum $q = |\mathbf{p} - \mathbf{p}'|$. It corresponds to the assumption of isotropy of the scattering process (i.e., azimuthal symmetry):

$$w_{QQ'}(\mathbf{r}, \mathbf{p}, \mathbf{q}) = w_{QQ'}(\mathbf{r}, |\mathbf{p} - \mathbf{p}'|).$$

Thus, the kinetic equations describing diffusion and charge exchange processes of channeled ions in space of transverse momenta in a single-electron approximation can be written as follows:

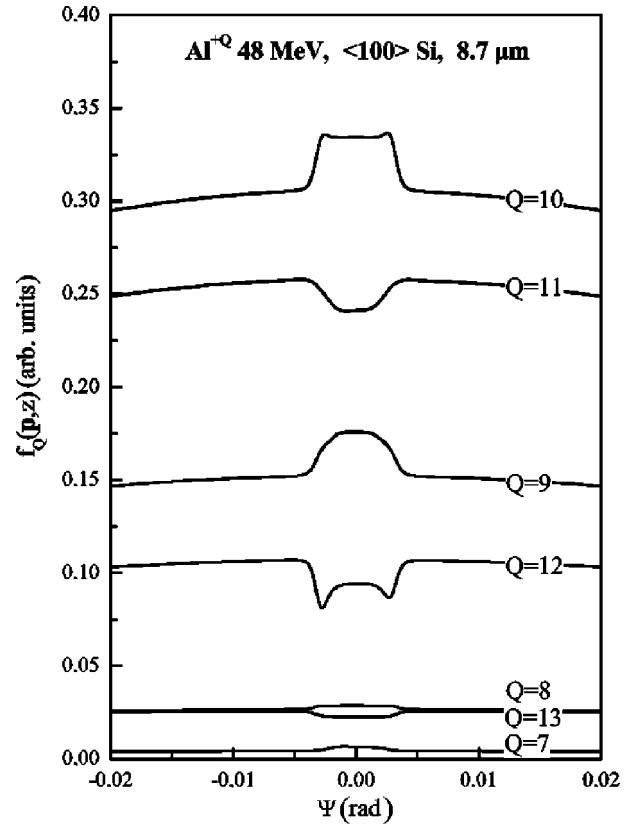


FIG. 5. Calculated partial axial angular distributions after transmission of an 8.7 μm Si $\langle 100 \rangle$ crystal given by different ion charge states.

$$\begin{aligned} \frac{\partial f_Q(\mathbf{p}, z)}{\partial z} = & \text{div}[\mathbf{A}_Q(\mathbf{p})f_Q(\mathbf{p}, z) + D_Q(\mathbf{p})\text{grad} f_Q(\mathbf{p}, z)] \\ & + \text{div}\{P_{Q-1}^l(\mathbf{p})[\mathbf{A}_Q(\mathbf{p})f_{Q-1}(\mathbf{p}, z) + D_Q(\mathbf{p})\text{grad} f_{Q-1}(\mathbf{p}, z)]\} \\ & + \text{div}\{P_{Q+1}^c(\mathbf{p})[\mathbf{A}_Q(\mathbf{p})f_{Q+1}(\mathbf{p}, z) + D_Q(\mathbf{p})\text{grad} f_{Q+1}(\mathbf{p}, z)]\} \\ & + [W_{Q+1,Q}(\mathbf{p})f_{Q+1}(\mathbf{p}, z) + W_{Q-1,Q}(\mathbf{p})f_{Q-1}(\mathbf{p}, z) - W_{Q,Q-1}(\mathbf{p})f_Q(\mathbf{p}, z) - W_{Q,Q+1}(\mathbf{p})f_Q(\mathbf{p}, z)]. \end{aligned} \quad (12)$$

The kinetic coefficients are determined by

$$D_Q(\mathbf{p}) = \frac{1}{4} \int \mathbf{q}^2 w_Q^{(1)}(\mathbf{p}, \mathbf{q}) d^2q, \quad (13)$$

$$\mathbf{A}_Q(\mathbf{p}) = \frac{\partial}{\partial \mathbf{p}} D_Q(\mathbf{p}). \quad (14)$$

The first term in the right part of the Eq. (12) represents the usual Fokker-Plank equation for the distribution function of charge state Q in space of transverse momenta. The second and the third terms describe the processes of the “generalized” diffusion at which there is a change of a transverse momentum due to multiple scattering and change of a

charge state of an ion. Last term in the right part of Eq. (12) represents the usual balance equation on charge states.

To formulate a nonstationary boundary-value problem, one needs to impose some initial and boundary conditions. We shall define the initial function $f_Q(\mathbf{p}, z=0)$ as a quasiuniform distribution on transverse momentum and equilibrium distribution on charge states (Ref. 3). Such initial conditions correspond to the conditions of the experiments.⁵⁻¹⁰ A boundary condition must take into account the reverse process from the above-barrier beam component to the under-barrier one. It is possible to define it as (see, for example, Ref. 19) $f_Q(\mathbf{p}^b, z)=0$, where $\mathbf{p}^b \approx K\mathbf{p}_{Q_{\max}}^c$ ($K > 1$) is the boundary momentum and $\mathbf{p}_{Q_{\max}}^c$ is a value of the Lindhard critical momentum¹¹ for ion charge state $Q_{\max}=Z_1$.

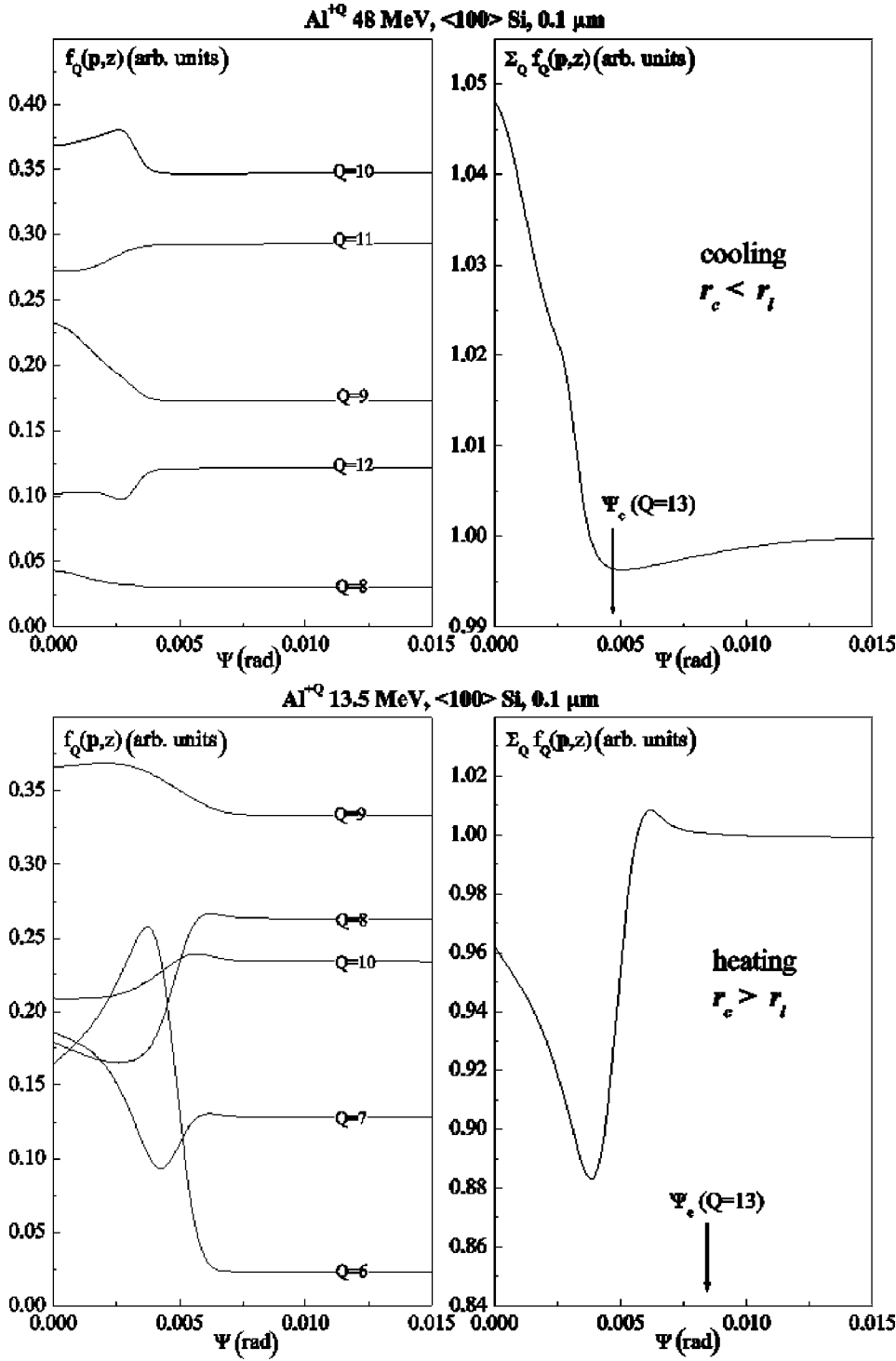


FIG. 6. Calculated full (right) and partial (left) axial angular distributions of Al^{+Q} ions after transmission of a 0.1 μm Si <100>, where $\Psi_c(Q=13)$ is the Lindhard angle for axial channeling at initial ion energy and charge state, $Q=13$.

The distribution function allows one to obtain a fraction of the above-barrier and the under-barrier ions in charge state Q at the depth z :

$$F(Q,z) = \int_S f_Q(\mathbf{p},z) d^2p, \quad (15)$$

where the integration area S on transverse momentum is limited from above by the critical momentum p_Q^c for under-barrier ions and from below for above-barrier ones:

$$p^2/2M_1 < (p_Q^c)^2/2M_1 \quad (\text{under-barrier}), \quad (16)$$

$$p^2/2M_1 \geq (p_Q^c)^2/2M_1 \quad (\text{above-barrier}). \quad (17)$$

It is convenient to consider the normalized distribution of charge states $N(Q,z)$ and an average charge $Q(z)$ for under-barrier and above-barrier ions:

$$N(Q,z) = \frac{F(Q,z)}{\sum_Q F(Q,z)}, \quad Q(z) = \sum_Q QN(Q,z). \quad (18)$$

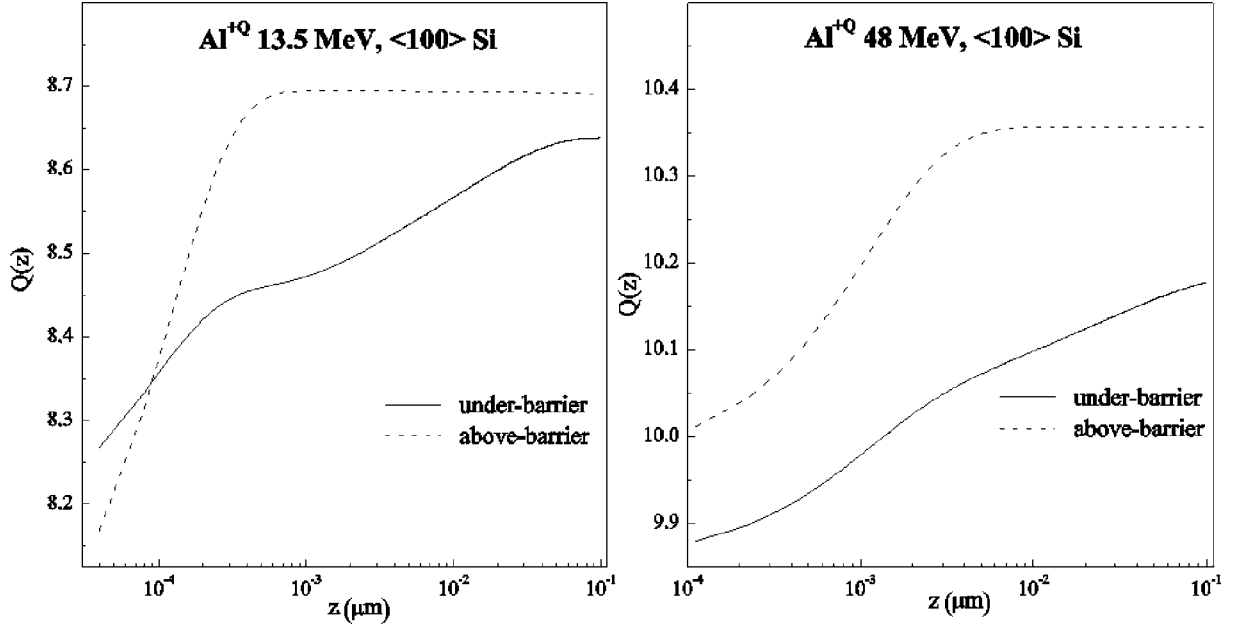


FIG. 7. Dependence of the mean charge $Q(z)$ on the penetration depth for under-barrier and above-barrier Al^{+Q} ions in a Si $\langle 100 \rangle$ crystal.

The angular distribution of ions transmitted through the crystal will be defined by the sum of partial charge states distribution:

$$f(\mathbf{p}, z) = \sum_Q f_Q(\mathbf{p}, z).$$

III. KINETIC COEFFICIENTS

A. Diffusion coefficients

According to Eqs. (2) and (13), the diffusion coefficients in Eq. (12) can be defined as average over an accessible area of that dependent on transverse coordinate diffusion coefficients:

$$D_Q(\mathbf{p}) = \frac{1}{S_Q(\mathbf{p})} \int_{S_Q(\mathbf{p})} D_Q(\mathbf{r}) d^2r, \quad (19)$$

$$D_Q(\mathbf{r}) = \frac{1}{4} \int \mathbf{q}^2 w_{QQ}(\mathbf{r}, \mathbf{q}) d^2q. \quad (20)$$

The diffusion processes are caused by scattering with electrons and lattice vibrations, i.e.,

$$D_Q(\mathbf{r}) = D_Q^e(\mathbf{r}) + D_Q^l(\mathbf{r}).$$

The diffusion coefficients $D_Q^e(\mathbf{r})$ and $D_Q^l(\mathbf{r})$ are calculated according to Ref. 20. The calculated values (13) of $D_Q(\mathbf{p})$ for Al^{+Q} ions channeled in a Si crystal along the $\langle 100 \rangle$ axial directions are shown in Fig. 1. At small transverse momentum the scattering by electrons is the determining factor of the diffusion. At an increase of transverse momentum, the accessible area of the channeling comes nearer to atomic

chains and prevailing there is the scattering by a nucleus. A further increase of the transverse momentum does not lead to the increase of the accessible area, and kinetic coefficients for above-barrier ions are constants.

B. Capture and loss probabilities

The calculation of probabilities $P_Q^{c,l}(\mathbf{p})$ is a difficult problem. For our purposes it is possible to use the empirical formulas for the capture and loss probabilities. Following Ref. 13 we have, for probabilities of electron capture and loss by an ion,

$$P_Q^c(\mathbf{r}) = \left[1 + \frac{2}{\pi} \arctan \left(\frac{\pi}{2} \alpha (Q - Q_0) \right) \right] \times \sum_s \int f^c(\mathbf{r}_s + \mathbf{u} - \mathbf{r}) \Phi(\mathbf{u}) d^2u,$$

$$P_Q^l(\mathbf{r}) = \left[1 - \frac{2}{\pi} \arctan \left(\frac{\pi}{2} \alpha (Q - Q_0) \right) \right] \times \sum_s \int f^l(\mathbf{r}_s + \mathbf{u} - \mathbf{r}) \Phi(\mathbf{u}) d^2u,$$

where Q_0 is the average charge in equilibrium for a random ion, \mathbf{r}_s is the atomic chain coordinate in the transverse plane, \mathbf{u} is the value of the transverse thermal vibration, and $\Phi(\mathbf{u})$ is the thermal distribution of the crystal atoms in the transverse plane. The functions $f^c(\mathbf{r}_s + \mathbf{u} - \mathbf{r})$ and $f^l(\mathbf{r}_s + \mathbf{u} - \mathbf{r})$ are given by¹³

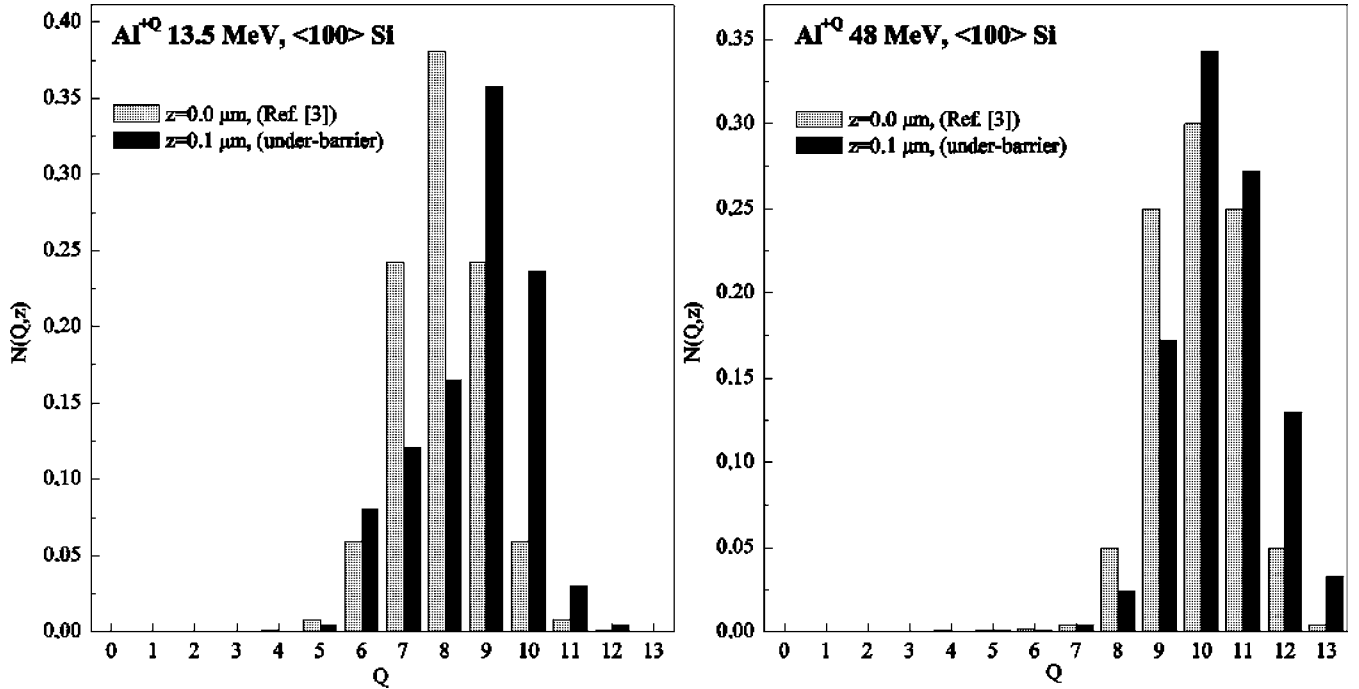


FIG. 8. Normalized distribution on charge states $N(Q, z)$ for under-barrier Al^{+Q} ions in a Si $\langle 100 \rangle$ crystal.

$$f^c(\mathbf{r}_s + \mathbf{u} - \mathbf{r}) = \theta(r_c - |\mathbf{r}_s + \mathbf{u} - \mathbf{r}|),$$

$$f^l(\mathbf{r}_s + \mathbf{u} - \mathbf{r}) = \frac{r_c^2}{2r_l^2} \exp(-|\mathbf{r}_s + \mathbf{u} - \mathbf{r}|/r_l),$$

where $\theta(x)=1$ if $x \geq 0$, and $\theta(x)=0$ if $x < 0$.

By adjusting the values of α and Q_0 we reproduce the distribution given by Ref. 3 for ion penetrating a carbon foil. The values of impact parameters for electron capture r_c and loss r_l are adjusted according to Refs. 1 and 13. The capture of an electron takes place at a distance from an atom less than a capture radius r_c .¹ The electron loss probability decreases exponentially at large impact parameters with a characteristic width close to the adiabatic distance r_l .¹³ Values obtained by this ansatz for Al^{+Q} ions with initial energies 13.5 and 48 MeV are given in Table I. The dependence of the capture and loss probabilities on a transverse momentum (9) for channeled Al^{+Q} ions along $\langle 100 \rangle$ direction in a Si crystal is shown in Fig. 2.

C. Length of free path

Similarly to the calculation of diffusion coefficients, we shall represent the length of the free path as an average over an accessible area,

$$1/L_Q(\mathbf{p}) = \frac{1}{S_Q(\mathbf{p})} \int_{S_Q(\mathbf{p})} d^2r \int w_{QQ}(\mathbf{r}, \mathbf{q}) d^2q. \quad (21)$$

The integral on a transferred transverse momentum in Eq. (21) is estimated by the expression

$$\int w_{QQ}(\mathbf{r}, \mathbf{q}) d^2q = \sigma_Q^{(e)} N_e(\mathbf{r}) + \sigma_Q^{(n)} N_n(\mathbf{r}), \quad (22)$$

where $\sigma_Q^{(e)}, \sigma_Q^{(n)}$ are the full cross sections of the excitation of valent electrons and elastic scattering by atoms of a crystal, respectively, $N_e(\mathbf{r})$ is the distribution of electron density in the crystal channel that can be found from the potential distribution in accordance with the Poisson equation, $N_n(\mathbf{r})$ is the distribution of atoms in the transverse plane due to thermal vibrations. The free pathlengths depending on transverse momentum for channeled Al^{+Q} ions along the $\langle 100 \rangle$ direction in a Si crystal are shown in Fig. 3.

IV. RESULTS AND DISCUSSION

The diffusion coefficients actually have first-order breaks (see Fig. 1) at values of transverse momentum near the critical one. Therefore, there are no simple numerical algorithms for a solution of the kinetic equation (12). The most effective and reliable method in this case is the integrointerpolation technique. The calculations were carried out for the penetration of a quasiuniform Al^{+Q} ion beam in a Si crystal along the axis $\langle 100 \rangle$ at various values of the projectiles energy. The potential in a transverse plane has been calculated as a superposition of continuous potentials of atomic chains. The Moliere approximation for the potential of an isolated atomic chain has been used.

The results of the solution of Eq. (12) for Al^{+Q} ions with energy 48 MeV and crystal thickness $8.7 \mu\text{m}$ are shown in Fig. 4. The central maximum (cooling effect) in the angular distribution of ions transmitted through the crystal breaks the isotropy of the angular distributions. It is caused by the processes of electron capture and loss. In order to check the role

of the charge exchange processes, (12) has been solved with the assumption $P_Q^{c,l}(\mathbf{p})=0$. In this case the solution does not lead to isotropy breaking of an initially isotropic ion beam [the surface (2) in Fig. 4]. It specifies the main role of charge exchange processes in the observed cooling effect.

In Ref. 5, the cooling effect at the transmission of Al^{+Q} ions through a Si crystal along the axial direction $\langle 100 \rangle$ was experimentally observed. Our calculations qualitatively confirm and explain the observed effect. The value of the cooling maximum in the calculations appears a little bit less than the experimental value. Probably, it is connected with the distinction of real probabilities of electron capture and loss from the empirical formulas we used.

Let us notice that the angular distribution shown in Fig. 4 (the surface (1)) is a superposition of the partial distributions of each charge states Q . The angular distributions of the various charge states are shown in Fig. 5. It is interesting to note that the angular distributions of the charge states with $Q=7, 8, 9$, and 10 contain a cooling maximum, and charge states with $Q=11, 12$, and 13 contain a heating minimum. The common feature of charge states with $Q=7, 8, 9$, and 10 is the large value of the electron loss probability in comparison with the capture probability in the above-barrier area. And the common feature of charge states $Q=11, 12$, and 13 is the small value of the electron loss probability, in comparison with the capture probability, in the above-barrier area. So, we come to a conclusion, that there is a tendency to cooling processes if the average charge in the above-barrier area is larger than the average charge in the under-barrier area. And there is a tendency to heating processes if the average charges in the above-barrier area are less than the average charges in the under-barrier areas. In Ref. 14 the transmission of a “two-charge state” beam of C^{+Q} ions through an oriented Si crystal was studied by computer simulation and a similar conclusion has been made. The “two-charge state” model is suitable for a C^{+Q} ion beam, as practically only two-charge states are populated for these ions according to Ref. 3. However, it is necessary to note that since the resulting angular distribution is a superposition of all charge states, the final angular distribution may differ strongly from the “two-charge state” model for other ion beams (see later).

The characteristic impact parameter of electron capture r_c is less than the characteristic impact parameter of electron loss r_l at the ion energy 48 MeV (see Table I). According to the qualitative speculations in Ref. 5 such a ratio should result in a cooling effect. And it proves to be true by the statistical theory (Fig. 4). At an ion energy of 13.5 MeV, we have $r_c > r_l$ (see Table I). According to the hypothesis of Ref. 5, in this case a heating effect should be observed. The results of the solution of Eq. (12) for these conditions are shown in Fig. 6. For comparison, the results of the calculations for energy 48 MeV are given in Fig. 6 as well. Thus, if $r_c < r_l$, it will induce transverse cooling and, conversely, if $r_c > r_l$, it will induce transverse heating. The overall heating

or cooling efficiency is high if r_c and r_l differ significantly. The angular distribution at energy 13.5 MeV is quite complex. In general, a heating effect is observed, but with cooling in the central part of angular distribution. The central cooling maximum is caused by the contribution of the charge state with $Q=7$.

Similar angular distributions have been observed experimentally in Refs. 8–10. The structure of the angular distribution strongly depends on the partial contribution of the various charge states. Since the angular distributions can be very different for different charge states, the structure of the total distribution can be rather nontrivial.

The dependence of the average ion charge on the depth of penetration into a crystal and the normalized distribution of charge states (18) are shown in Figs. 7 and 8. The equilibrium charge in the above-barrier area for 48 and 13.5 MeV is equal to 10.4 and 8.7, respectively. The ion charge reaches the equilibrium values at slightly larger depths of penetration in the under-barrier area. These values are smaller than the above-barrier equilibrium charge for both energies. Nevertheless, a heating minimum in the angular distribution is present at the ion energy 13.5 MeV and a cooling maximum at the energy 48 MeV. So, as it was specified previously, the final angular distribution differs from the prediction of the “two-charge state” model because the resulting angular distribution is a superposition of all charge states. The occurrence of cooling or heating effects and the detailed structure of the angular distribution depend on both the impact parameter dependence of the probabilities for electron capture and loss and on the relative contributions from different charge states.

The normalized distributions of charge states (Fig. 8) realize the common features of the under-barrier ions. The maximum of the distribution is displaced to large charges and the structure of the distribution differs significantly from the Poisson distribution.

Thus, the developed statistical theory, which takes into account the diffusion of ions in transverse momentum and charge exchange processes, adequately describes observable angular distributions of multicharge heavy ions scattered by a crystal. The statistical theory allows us to calculate the partial angular distributions of various charge states and to explain the physical nature of a cooling maximum or a heating minimum in the angular distributions. For the quantitative description of the observed features, it is necessary to know the details of the dependence of the capture and loss probabilities on the impact parameter. By comparing the measured and the calculated angular distributions, one can determine precisely the impact parameter dependence of the capture and loss processes for all charge states. A further development of the experimental methods and theory can result in the creation of a new effective tool in the channeling technique for studying ion-atom collisions in solids.

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