Rainbow effect in ion channeling

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The problem of ion channeling in very thin crystals is considered with use of a method of classical ion-molecule scattering theory complemented with the Monte Carlo method. Special attention is devoted to the rainbow effect. It is shown that this effect is a consequence of the fact that contributions of the atomic strings of the crystal to the probability of ion transmission interfere. In the calculations the projectiles were 7-MeV H^+ ions, and they were being transmitted through the $\langle 110 \rangle$ channel of a $\cong$1500-Å-thick Si crystal; the case in which the incident energy is 10 MeV and crystal thickness $\cong$1000 Å is also analyzed. The effect of thermal vibrations of the atoms of the crystal and the effect of collisions of the ion with the electrons of the crystal are taken into account.

I. INTRODUCTION

Theoretical investigations of the problem of ion channeling in crystals have been developed along two major lines. The first one is based on the analytical approach of Lindhard,[1] which uses the methods of statistical mechanics, and includes the continuum approximation and the assumption of statistical equilibrium in the transverse plane. The last assumption makes the approach valid only for thick crystals. It is important to note that within that treatment the effect of correlations between the atomic strings of the crystal, i.e., the effect of transverse correlations, it not taken into account. The second line of investigation is based on the Monte Carlo approach in which trajectories of the ions through the crystal are followed.[2] We would also like to mention the calculations of Golovchenko,[3] and Ellison *et al.*[4] Their approaches are with the methods of statistical mechanics, but without the assumption of statistical equilibrium in the transverse plane. Thus they can be used for thin crystals. The former treatment is analytical while the latter is, in general, numerical. Besides, Golovchenko did not and Ellison *et al.* did take into account the effect of transverse correlations.

The treatment of ion channeling to be presented in this paper is valid only for very thin crystals. It uses a method of the ion-molecule scattering theory and the Monte Carlo method. The approach is based on the (classical) momentum approximation, within which the effect of correlations between the atoms of one atomic string of the crystal, i.e., the effect of longitudinal correlations, is neglected. However, the approximation enables a proper treatment of the effect of transverse correlations. The ion-molecule scattering theory is used to analyze the probability of ion transmission as a function of the impact parameter. The Monte Carlo method is used to obtain the angular distribution of the transmitted ions. When compared to the trajectory following Monte Carlo calculations, this calculation is less accurate, but its simplicity enables one to work with a much greater number of ions, and thus achieve a substantially better angular resolution.

II. THEORY

Let us take the z axis to coincide with the channel axis and the origin to lie in the median plane of the crystal. The incident velocity of the ion is parallel to the z axis. The crystal is assumed to be sufficiently thin for the ion trajectory to be approximated by a straight line, i.e., for the transverse motion of the ion to be ignored. In this case one can apply the momentum approximation. Within this approximation the x and y components of the scattering angle are the following:

$$\theta_x = -\frac{1}{2E}\sum_{i=1}^{M}\sum_{k=1}^{N}\int_{-\infty}^{\infty}\partial_x U_{ik}\,dz$$

and (1)

$$\theta_y = -\frac{1}{2E}\sum_{i=1}^{M}\sum_{k=1}^{N}\int_{-\infty}^{\infty}\partial_y U_{ik}\,dz\ ,$$

where E is the incident energy, $U_{ik}=U_{ik}(x,y,z)$ the interaction potential of the ion and the kth atom of the ith atomic string of the crystal, M the number of atomic strings, and N the number of atoms in one string; $\partial_x \equiv \partial/\partial_x$ and $\partial_y \equiv \partial/\partial_y$. These expressions show that from the point of view of components of the scattering angle the $(MN+1)$-particle collision under consideration reduces to MN independent two-particle collisions, i.e., the effect of multiple scattering can not be observed.[5] It is clear that contributions of the atoms of one atomic string to the components of the scattering angle do not depend on their positions within the string, and thus

$$\theta_x = -\frac{N}{2E}\sum_{i=1}^{M}\partial_x V_i$$

and (2)

$$\theta_y = -\frac{N}{2E}\sum_{i=1}^{M}\partial_y V_i\ ,$$

where $V_i = V_i(x,y)$ is the integral along the trajectory of the interaction potential of the ion and one of the atoms of the ith atomic string. These expressions show that the

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process we analyze in fact consists (from the point of view of components of the scattering angle) of M independent two-particle collisions. Thus applying the momentum approximation we neglect the fact that the atoms of one atomic string are arranged in a nonrandom way, i.e., the effect of longitudinal correlations.

In the case under consideration the differential scattering cross section is

$$\sigma = |J|^{-1} ,$$

where (3)

$$J = \partial_x \theta_x \partial_y \theta_y - \partial_y \theta_x \partial_x \theta_y$$

[J is the Jacobian of functions $\theta_x(x,y)$ and $\theta_y(x,y)$].[6,7] We may call this cross section the differential-transmission cross section. Variable J can be expressed as

$$J = J_0 + J' , \tag{4}$$

where

$$J_0 = \sum_{i=1}^{M} J_{ii}, \quad J' = \sum_{i=1}^{M} \sum_{j=i+1}^{M} (J_{ij} + J_{ji}) \tag{5}$$

and

$$J_{ij} = \left[\frac{N}{2E} \right]^2 (\partial_{xx} V_i \partial_{yy} V_j - \partial_{xy} V_i \partial_{xy} V_j) . \tag{6}$$

Term J_{ii} describes the scattering from the ith atomic string of the crystal, and the sum of terms J_{ij} and J_{ji} describes the coupling between the ith and jth atomic strings as seen by the ion. Hence, from the point of view of differential-transmission cross section the $(MN+1)$-particle collision in question does not reduce the MN independent two-particle collisions, i.e., the effect of multiple scattering can be observed.[5] In this case the process we analyze consists of M nonindependent two-particle collisions. We want to emphasize that this is an interference effect: Contributions of the atomic strings to the differential-transmission cross section interfere.

It is obvious that the equation $J'=0$ defines the line along which the effect of multiple scattering is not observable.[5] We may call this line the single-scattering line. The rainbow line, i.e., the line along which the differential-transmission cross section is infinite,[6,7] is given by the equation $J=0$. These lines are defined in the impact parameter plane or in the scattering angle plane.

Let us now introduce the effect of thermal vibrations of the atoms of the crystal. This will be done by averaging variable V_i over the transverse displacements of the atom from its equilibrium position.[8] The displacements of the atom along the x and y axes are taken to be small and independent; they are described by the Gaussian distribution function. Consequently, one can obtain

$$V_i^{\text{th}} = V_i + \frac{\sigma_{\text{th}}^2}{2} (\partial_{xx} V_i + \partial_{yy} V_i) , \tag{7}$$

where σ_{th} is the standard deviation of the distribution, i.e., the one-dimensional thermal-vibration amplitude. The components of the scattering angle and the differential-transmission cross section are now given by Eqs. (2)—(6) with variable V_i replaced by V_i^{th}.

We shall also take into account the effect of collisions of the ion with the electrons of the crystal. These collisions cause an uncertainty of the scattering angle of the ion.[1] In our case the average square uncertainty of the scattering angle is[1]

$$\sigma_e^2 = \frac{\pi Z_1^2 e^4 (N-1)c}{E^2} n_e L_e , \tag{8}$$

where Z_1 is the atomic number of the ion, e the unit charge, c the distance between the atoms of the atomic strings of the crystal, and n_e the average density of the electrons of the crystal along the straight line parallel to the channel axis and determined by the average position of the ion in the transverse plane; L_e is a function of the incident velocity and density n_e, and we shall use for it the expression valid in the case in which the ion velocity is much greater than the maximal velocity of the electrons of the crystal.[9] With the assumption that the components of the scattering angle of the ion within the crystal are linear functions of time the average position of the ion in the transverse plane is given by

$$x' = x + \frac{(N-1)c}{6} \theta_x$$

and (9)

$$y' = y + \frac{(N-1)c}{6} \theta_y .$$

In this analysis we shall assume that the ion-atom interaction potential is of the Thomas-Fermi type, and for the integral of that potential along the trajectory we shall use Lindhard's expression[1]

$$V_i = Z_1 Z_2 e^2 \ln \left[\frac{C a_s^2}{p_i^2} + 1 \right] , \tag{10}$$

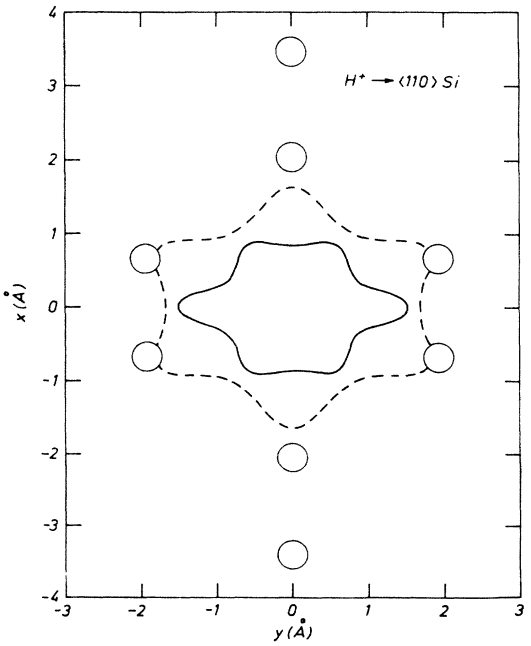

FIG. 1. The single-scattering line (dashed line) and the rainbow line (solid line) in the impact parameter plane.

where Z_2 is the atomic number of the crystal, a_s is the screening length, $p_i^2=(x-x_i)^2+(y-y_i)^2$, x_i and y_i are the coordinates of the ith atomic string of the crystal, and $C=3$ is a fitting parameter.

III. RESULTS AND DISCUSSION

Let us now concentrate on the transmission of H^+ ions through the $\langle 110\rangle$ channel of a Si crystal. The incident energy will be 7 MeV, and the crystal will be $\cong 1500$ Å thick ($N=392$). Figure 1 shows the single-scattering line and the rainbow line in the impact parameter plane in this $H^+ \rightarrow$Si case. The number of atomic strings of the crystal (M) is 20, i.e., we took into account the strings lying on the four nearest (relative to the channel axis) coordination circles; the effect of thermal vibrations of the atoms of the crystal is not taken into account. It is clear that the single-scattering line connects the regions of the impact parameter plane in which the scattering process under consideration is dominated by the interaction with one atomic string. It can be said that this line is "attracted" by the strings defining the channel. On the other hand, the rainbow line lies in the region of the impact parameter plane where the contributions of more atomic strings are important. This line is "repelled" by the strings defining the channel. It must be emphasized that the lines given in Fig. 1 are determined only by the arrangement of the atomic strings and the screening length; they do not depend on the incident energy and crystal thickness. The single-scattering line and the rainbow line have also been analyzed in the cases of 6, 8, and 12 atomic strings, i.e., one, two, and three coordination circles, respectively. The answer was that the strings lying on the second coordination circle influenced the shape of those lines, and that the contribution of those lying on the third and fourth coordination circles to the coordinates of the lines was small: less than $\cong 0.05$ Å.

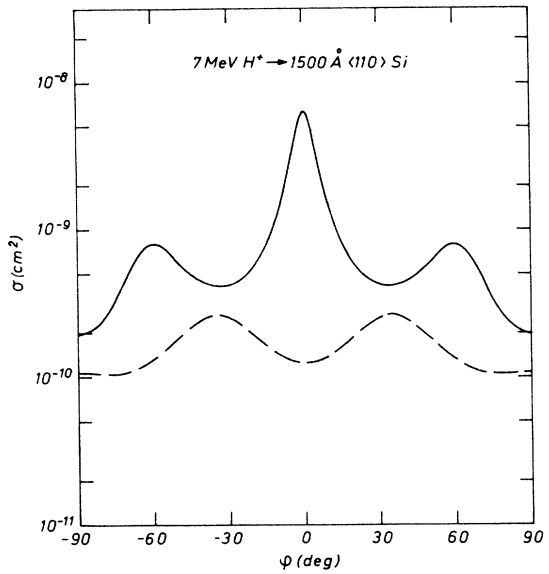

FIG. 3. The dependence of the differential-transmission cross section on variable ϕ for $\rho=0.850$ Å without (dashed line) and with (solid line) the effect of multiple scattering; the incident energy is 7 MeV and crystal thickness $\cong 1500$ Å.

Figures 2 and 3 give dependences of the differential-transmission cross section on variable $\rho=(x^2+y^2)^{1/2}$ for $\phi=\tan^{-1}(y/x)=30$ and 210°, and on variable ϕ for $\rho=0.850$ Å, respectively; the number of atomic strings of the crystal is 20, and the effect of thermal vibrations of

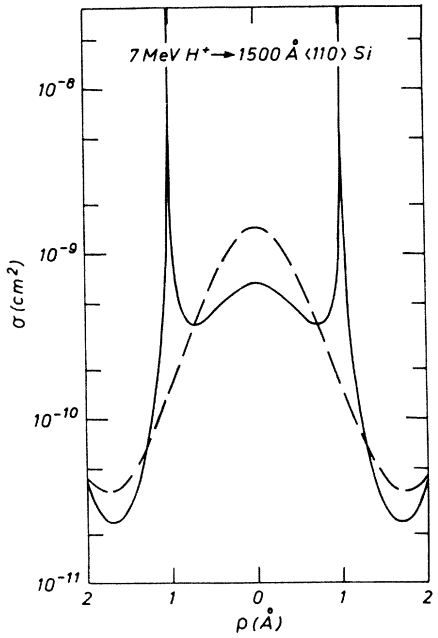

FIG. 2. The dependence of the differential-transmission cross section on variable ρ for $\phi=30$ and 210° without (dashed line) and with (solid line) the effect of multiple scattering; the incident energy is 7 MeV and crystal thickness $\cong 1500$ Å.

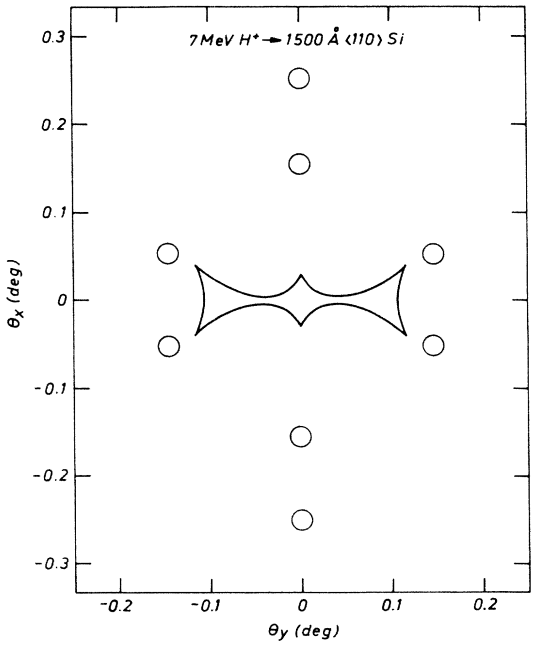

FIG. 4. The rainbow line in the scattering angle plane for the incident energy of 7 MeV and crystal thickness of $\cong 1500$ Å.

the atoms of the crystal is ignored. These figures also contain the differential-transmission cross section when term J' is not taken into account, i.e., when the effect of multiple scattering is neglected. The radial dependences of the differential-transmission cross section (Fig. 2) clearly demonstrate that the rainbow effect is a consequence of the multiple scattering, i.e., of the fact that contributions of the atomic strings to the differential-transmission cross section interfere. The azimuthal dependences of the differential-transmission cross section (Fig. 3) show that without the effect of multiple scattering this variable is maximal between the atomic strings and minimal towards them, what is also true for all other values of variable ρ, and that with this effect it can be maximal towards the atomic strings.

Now, we may examine the rainbow line in the scattering angle plane. It is shown in Fig. 4; the number of atomic strings of the crystal is 20, and the effect of thermal vibrations of the atoms of the crystal is not taken into account. The circles appearing in this figure represent the last atoms of the atomic strings lying on the first two coordination circles; the angles corresponding to these circles are determined by the z axis and the lines defined by the origin and these atoms. It is important to note that the approximation used (within which the transverse motion of the ion is neglected) does not give correct results in the vicinity of these circles. This is related to the extreme left and right parts of the rainbow line shown in this figure. Let us, therefore, from now one concentrate on the central part of the rainbow line, i.e., on the region in which the scattering angle is smaller than $\sim 0.03°$; the corresponding (maximal) distance traveled by the ion in the transverse plane is ~ 0.4 Å. It must be emphasized that the momentum approximation overestimates the scattering angle of the ion; a more accurate calculation would give smaller distances traveled by the ion in the transverse plane. For higher incident energies and/or thinner crystals the dimensions of the rainbow line are smaller [see Eqs. (2)]. For example, for the incident energy of 10 MeV and crystal thickness of $\cong 1000$ Å ($N=261$) the central part of the rainbow line lies in the region in which the scattering angle is smaller than $\sim 0.015°$; the corresponding distance traveled by the ion in the traverse plane is ~ 0.13 Å; in this case the six circles representing the atomic strings defining the channel lie on a circle of radius equal to 0.234°.

The next step is to analyze the influence of the effect of thermal vibrations of the atoms of the crystal. For parameter σ_{th} we took the value of 0.0744 Å corresponding to room temperature.[10] The calculation showed that changes of the coordinates of the rainbow line (Figs. 1 and 4) due to this effect were very small. For example, the singularity in the differential-transmission cross section shown in Fig. 2 shifted towards higher values of variable ρ by 0.001 Å. This agrees with the fact that the rainbow line in the impact parameter plane is "repelled" by the atomic strings of the crystal, and justifies the way in which the effect of thermal vibrations was introduced.

Let us now consider the angular distribution of the transmitted ions. It is given by Eqs. (3) and (2), i.e., by

$$\sigma = f[x(\theta_x,\theta_y), y(\theta_x,\theta_y)] = g(\theta_x,\theta_y) . \tag{11}$$

However, variables x and y are complicated multivalued functions of θ_x and θ_y.[7] Therefore, in order to avoid the mathematical difficulties, the Monte Carlo method was used. Values of variables x and y were chosen randomly within the region of the channel in the first quadrant of the impact parameter plane, and, according to the calculated values of θ_x and θ_y [Eqs. (2)], each particle was recorded as if it had entered a bin in the scattering angle plane; the number of atomic strings of the crystal was 8, while the number of ions was 5×10^5. In choosing variables x and y circular regions around the atomic strings with radii equal to the screening length were avoided, and thus the large values of the scattering angle were eliminated. The complete angular distribution of the transmitted ions was obtained using the fact that variables θ_x and θ_y are odd functions of x and y, respectively, and even func-

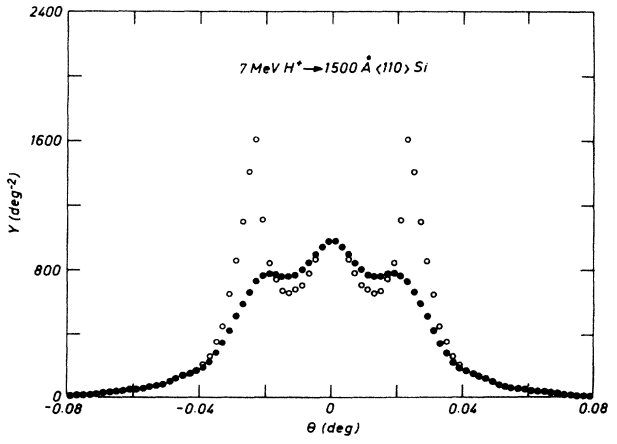

FIG. 5. The dependence of the yield of the transmitted ions on variable θ for $\Phi=0$ and 180° without (open circles) and with (closed circles) the effect of thermal vibrations and the effect of collisions with the electrons; the incident energy is 7 MeV and crystal thickness $\cong 1500$ Å.

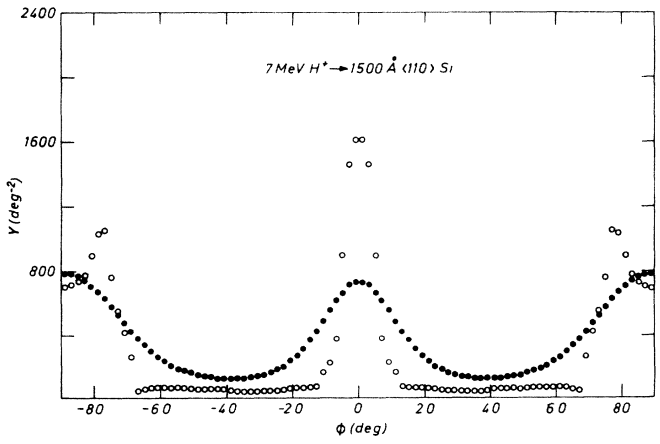

FIG. 6. The dependence of the yield of the transmitted ions on variable Φ for $\theta=0.023°$ without (open circles) and with (closed circles) the effect of thermal vibrations and the effect of collisions with the electrons; the incident energy is 7 MeV and crystal thickness $\cong 1500$ Å.

tions of y and x, respectively. Figures 5 and 6 give dependences of the yield of the transmitted ions on variable $\theta=(\theta_x^2+\theta_y^2)^{1/2}$ for $\Phi=\tan^{-1}(\theta_y/\theta_x)=0$ and 180°, and on variable Φ for $\theta=0.023°$, respectively; the sizes of the bin along the θ_x and θ_y axes are equal to 0.002°; the effect of thermal vibrations of the atoms of the crystal is neglected. The calculation in which this effect is included [using Eqs. (2) and (7)] shows that its influence is very small: The widths of the peaks corresponding to the rainbow effect virtually does not change. These figures also contain the corresponding yields of the transmitted ions when the effect of thermal vibrations and the effect of collisions of the ion with the electrons of the crystal are taken into account. The new angular distribution of the transmitted ions is a sum of the two-dimensional Gaussian distribution functions located at the centers of the bins; the dispersion of the distribution corresponding to one particular bin is equal to the average of variable σ_e^2 within the bin; the new distribution is normalized to the old one at the origin. It is evident that for the chosen values of the incident energy and crystal thickness the smearing of the rainbow effect caused by the collisions with the electrons is significant, and that it is more pronounced in the case of radial dependence of the yield of the transmitted ions (Fig. 5). The azimuthal dependences of the yield of the transmitted ions (Fig. 6) show that with the effect of collisions with the electrons the rainbow line looks as if it has four points, each of them directed towards a pair of atomic strings of the crystal. It is clear that in a more accurate calculation, which would take into account the transverse motion of the ion, the rainbow effect will be additionally smeared.

We have also analyzed the angular distribution of the transmitted ions for the incident energy of 10 MeV and crystal thickness of $\cong 1000$ Å. In this case the smearing of the rainbow effect due to the collisions of the ion with the electrons of the crystal is more pronounced than in the case of 7 MeV and $\cong 1500$ Å. This is in accordance with the fact that ratio of variables σ_e and θ is greater for higher incident energies and thinner crystals [see Eqs. (8) and (2)].[9] In the case of radial dependence of the yield of the transmitted ions the peaks corresponding to the rainbow effect virtually disappear. However, the azimuthal dependences of the yield of the transmitted ions show that the rainbow effect could be observed with these values of the incident energy and crystal thickness. This is illustrated in Fig. 7. The number of atomic strings of the crystal was 8, the number of ions was 5×10^5, and the sizes of the bin along the θ_x and θ_y axes were 0.001°. The value of variable θ is 0.0105°. For these values of the incident energy and crystal thickness the smearing of the rainbow effect due to the transverse motion of the ion is less pronounced than in the case of 7 MeV and $\cong 1500$ Å (it has been said above that in this case the central part of the rainbow line in the scattering angle plane lies in the region in which the distance traveled by the ion in the transverse plane is smaller than ~ 0.13 Å).

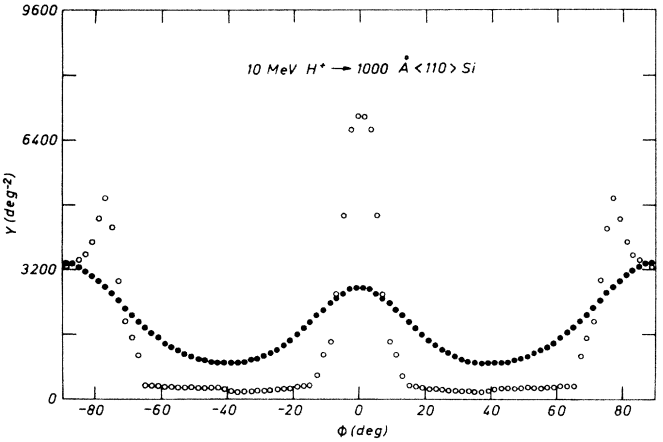

FIG. 7. The dependence of the yield of the transmitted ions on variable Φ for $\theta=0.0105°$ without (open circles) and with (closed circles) the effect of thermal vibrations and the effect of collisions with the electrons; the incident energy is 10 MeV and crystal thickness $\cong 1000$ Å.

We think that investigations of the rainbow effect in ion channeling could lead to a precise determination of the potential in crystal channels. Besides, it has been found that this effect could be important for processes including the internal degrees of freedom of channeled ions.[11] Namely, the fact that, besides the focusing corresponding to the channel center, there is an additional focusing of the ions clearly leads to a complex energy distribution of their electronic states.

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