# Theory of rainbows in thin crystals: The explanation of ion channeling applied to $Ne^{10+}$ ions transmitted through a ⟨100⟩ Si thin crystal

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(Received 5 October 1998; revised manuscript received 6 July 1999)

The theory of crystal rainbows is presented. It enables the generation and full explanation of the angular distribution of ions transmitted through thin crystals. The angular distribution of the transmitted ions is generated by the computer simulation method. Then, the rainbow lines in the scattering angle plane are determined. These lines ensure the full explanation of the angular distribution. The theory is applied to the transmission of $Ne^{10+}$ ions through a ⟨100⟩ Si thin crystal. The ion energy is 60 MeV and the crystal thickness is varied from 105 to 632 atomic layers, i.e., from the beginning of the first rainbow cycle to the beginning of the second rainbow cycle.

## I. INTRODUCTION

Theoretical studies of ion channeling in crystals have been going on along two major lines. The first line was founded by Lindhard,[1] and the second one by Barrett.[2,3] Lindhard's approach was via statistical mechanics, and it was analytical. He included the continuum approximation, i.e., neglected the (longitudinal) correlations between the positions of the atoms of one atomic string of the crystal, neglected the (transverse) correlations between the positions of the atomic strings, and included the assumption of statistical equilibrium in the transverse plane. Barrett's approach was via the ion-atom scattering theory, and it was numerical. He developed a very realistic computer code for the three-dimensional following of ion trajectories in crystal channels, in which the three approximations used by Lindhard were avoided. Barrett's approach is more complex, but a number of calculations have shown that it is much more accurate than Lindhard's approach. The coincidence of the experimental and theoretical results obtained by Krause *et al.*[4] clearly demonstrates the accuracy of Barrett's approach. Lindhard's approach would give the angular distributions of the channeled ions which would be qualitatively different from the angular distributions obtained by Krause *et al.*

Lindhard's and Barrett's approaches are described in detail in the famous review article on channeling and related effects of Gemmell.[5] A brief description of Lindhard's approach can be found in the study of resonant electronic processes accompanying heavy ion channeling by Andersen *et al.*[6] Regarding Barrett's approach, we would like to mention here the following four studies and a review article relevant to this work. Abel *et al.*[7] calculated the distribution of 1.9 MeV $He^{+}$ ions in the {110} planar channel of a thin Fe crystal as a function of the crystal thickness using the continuum approximation. They demonstrated that the yield of the channeled ions near the channel center was periodic with respect to the crystal thickness. In addition, they found that the distribution of the channeled ions at the distance from the channel center which varied with the crystal thickness was singular. Smulders and Boerma,[8] and Dygo and Turos[9] developed the computer codes for the three-dimensional following of ion trajectories in crystal channels similar to Barrett's. Those codes were used to analyze the transition from the ⟨110⟩ axial channeling to the {211} planar channeling of 1 MeV $He^{+}$ ions in a thin Si crystal.[10] They observed a strong focusing effect in the transition region accompanied by the dramatic changes in the energy spectra of the ions. Krause and Datz[11] wrote an interesting review article on heavy ion channeling. It contains a brief description of the angular distributions of ions transmitted through thin crystals.

Nešković[12] showed theoretically that in the transmission of ions through axial channels of very thin crystals the rainbows occurred, i.e., that the corresponding differential transmission cross section could be singular. His approach was via the ion-molecule scattering theory, and it was numerical. In that approach the continuum approximation was included implicitly, the correlations between the positions of the atomic strings of the crystal were included, and the assumption of statistical equilibrium in the transverse plane was avoided. Shortly after the prediction, the crystal rainbow effect was observed.[13]

Krause *et al.*[4] studied the angular distributions of $6-30$ MeV $C^{(4-6)+}$ ions transmitted through a ⟨100⟩ Si thin crystal. They showed that the angular distributions of the transmitted ions could be classified by the reduced crystal thickness, and that some maxima of the angular distributions could be attributed to the crystal rainbows. The reduced crystal thickness is defined by expression

$$\Lambda = f(qe,m)L/v, \tag{1}$$

where $qe$, $m$, and $v$ are the ion charge, ion mass, and average ion velocity, $e$ is the elementary charge, $L$ is the crystal thickness, and $f(qe,m)$ is the average frequency of the transverse motion of the ions.[4,14] Also, it has been demonstrated that the evolution of the angular distribution with the reduced crystal thickness has a periodic behavior.[4,15–17] The values of variable $\Lambda$ equal to 0.0, 0.5, 1.0, . . . correspond to the beginnings of the cycles of the angular distribution. These cycles are called the rainbow cycles.[15] However, the evolution of the angular distribution with $\Lambda$ within one rainbow cycle, as well as the differences between the angular distributions in different rainbow cycles remained unexplained.

We shall present here the theory of the crystal rainbow, which is the generalization of the model introduced by Nešković.[12] This theory will be used to analyze the case of $Ne^{10+}$ ions and a ⟨100⟩ Si thin crystal. The ion energy will be 60 MeV and the crystal thickness will be varied from 105 to 632 atomic layers, i.e., from the beginning of the first rainbow cycle to the beginning of the second rainbow cycle. We shall compare the evolution of the angular distribution of the transmitted ions with the reduced crystal thickness with the evolution of the crystal rainbow.

## II. THEORY

The system under consideration is an ion moving through an axial channel of a thin crystal. We assume that the interaction of the ion and the crystal is elastic, and that it can be treated classically.[1] The $z$ axis coincides with the channel axis and the origin lies in the entrance plane of the crystal. The angle between the initial ion velocity vector and the $z$ axis is taken to be zero. However, the theory of the crystal rainbow can easily include the case in which this angle is not zero.

We assume that the ion-atom interaction potential is of the Thomas-Fermi type, and adopt for it Moliere's expression,

$$V(r)=(Z_1Z_2e^2/r)[0.35\exp(-br)+0.55\exp(-4br)+0.10\exp(-20br)], \tag{2}$$

where $Z_1$ and $Z_2$ are the atomic numbers of the ion and the atoms of the crystal, respectively, $r$ is the distance between the ion and the atom, $b=0.3/a$, $a=[9\pi^2/(128Z_2)]^{1/3}a_0$ is the screening radius of the atoms, and $a_0$ is the Bohr radius.[4,11] This expression is chosen following the excellent experience of Krause *et al.* with it[4,11] (who studied the angular distributions of the medium energy heavy ions transmitted through a ⟨100⟩ Si thin crystal too). We also assume that we can apply the continuum approximation.[1] For the continuum potential of the $i$th atomic string of the crystal we use expression

$$U_i^{\mathrm{th}}(x,y)=U_i(x,y)+(\sigma_{\mathrm{th}}^2/2)[\partial_{xx}U_i(x,y)+\partial_{yy}U_i(x,y)], \tag{3}$$

where $U_i(x,y)$ is the continuum potential of the $i$th atomic string with the thermal vibrations of the atoms neglected, $x$ and $y$ are the transverse components of the ion position, and $\sigma_{\mathrm{th}}$ is the one-dimensional thermal vibration amplitude of the atoms.[12] The continuum potential of the crystal is the sum of the continuum potentials of the atomic strings.

We shall neglect here the energy loss of the ion, the changes of its charge, and the uncertainty of its scattering angle caused by the collisions with the electrons of the crystal. However, these effects can be included in the theory of the crystal rainbow.[12]

In order to obtain the components of the scattering angle of the ion, $\Theta_x$ and $\Theta_y$, one has to solve the equations of motion of the ion in the transverse plane, and use expressions $\Theta_x=V_x/V_0$ and $\Theta_y=V_y/V_0$, where $V_x$ and $V_y$ are the transverse components of the final ion velocity, and $V_0$ is the initial ion velocity. The angular distribution of the transmitted ions is generated by the computer simulation method.[2,3,14–17] The transverse components of the initial ion position, i.e., the components of its impact parameter, are chosen randomly or uniformly within the region of the channel.

Alternatively, instead of solving the equations of motion of the ion in the transverse plane, the components of its scattering angle can be obtained after the three-dimensional following of its trajectory, as in Barrett's approach.[2,3] In that case the continuum approximation is avoided.

The scattering law of the ion is given by expressions

$$\Theta_x=\Theta_x(x_0,y_0;\Lambda) \quad \text{and} \quad \Theta_y(x_0,y_0;\Lambda), \tag{4}$$

where $x_0$ and $y_0$ are the components of the impact parameter of the ion.

Since the scattering angle of the ion is small, the expression for its differential transmission cross section is

$$\sigma=1/|J|, \tag{5}$$

where $J=J(x_0,y_0;\Lambda)$ is the Jacobian of the components of the scattering angle, which describes the mapping of the impact parameter plane to the scattering angle plane in the process under consideration.[12,13]

Thus, the rainbow lines in the impact parameter plane, i.e., the lines in the impact parameter plane along which the differential transmission cross section of the ion is singular, are determined by equation

$$J(x_0,y_0;\Lambda)=0. \tag{6}$$

The rainbow lines in the scattering angle plane are determined by Eqs. (6) and (4), i.e., they are the images of the rainbow lines in the impact parameter plane, defined by the scattering law of the ion.

It should be noted that in the model introduced by Nešković[12] the components of the scattering angle and the differential transmission cross section of the ion, as well as the rainbow lines in the impact parameter plane and the shapes of the rainbow lines in the scattering angle plane depend only on the components of the impact parameter of the ion.

It will be shown here that the determination of the rainbow lines in the scattering angle plane is crucial for the explanation of the angular distribution of the transmitted ions. This step had not been included in Barrett's approach,[2,3] and, hence, it could not ensure the full explanation of the angular distributions obtained by Krause *et al.*[4]

## III. RESULTS AND DISCUSSION

As we have already said, we shall analyze here the angular distributions of $Ne^{10+}$ ions transmitted through a ⟨100⟩ Si thin crystal. The ion energy will be 60 MeV and the crystal thickness will be varied from 105 to 632 atomic layers; the thickness of one atomic layer is 0.543 082 nm.[18] This range corresponds to the range of the reduced crystal thickness from 0.10 to 0.60, i.e., from the beginning of the first rainbow cycle to the beginning of the second rainbow cycle. The one-dimensional thermal vibration amplitude of the atoms of the crystal is 0.007 44 nm.[19] We assume that the atomic strings defining the channel lie on the $x$ and $y$ axes. The

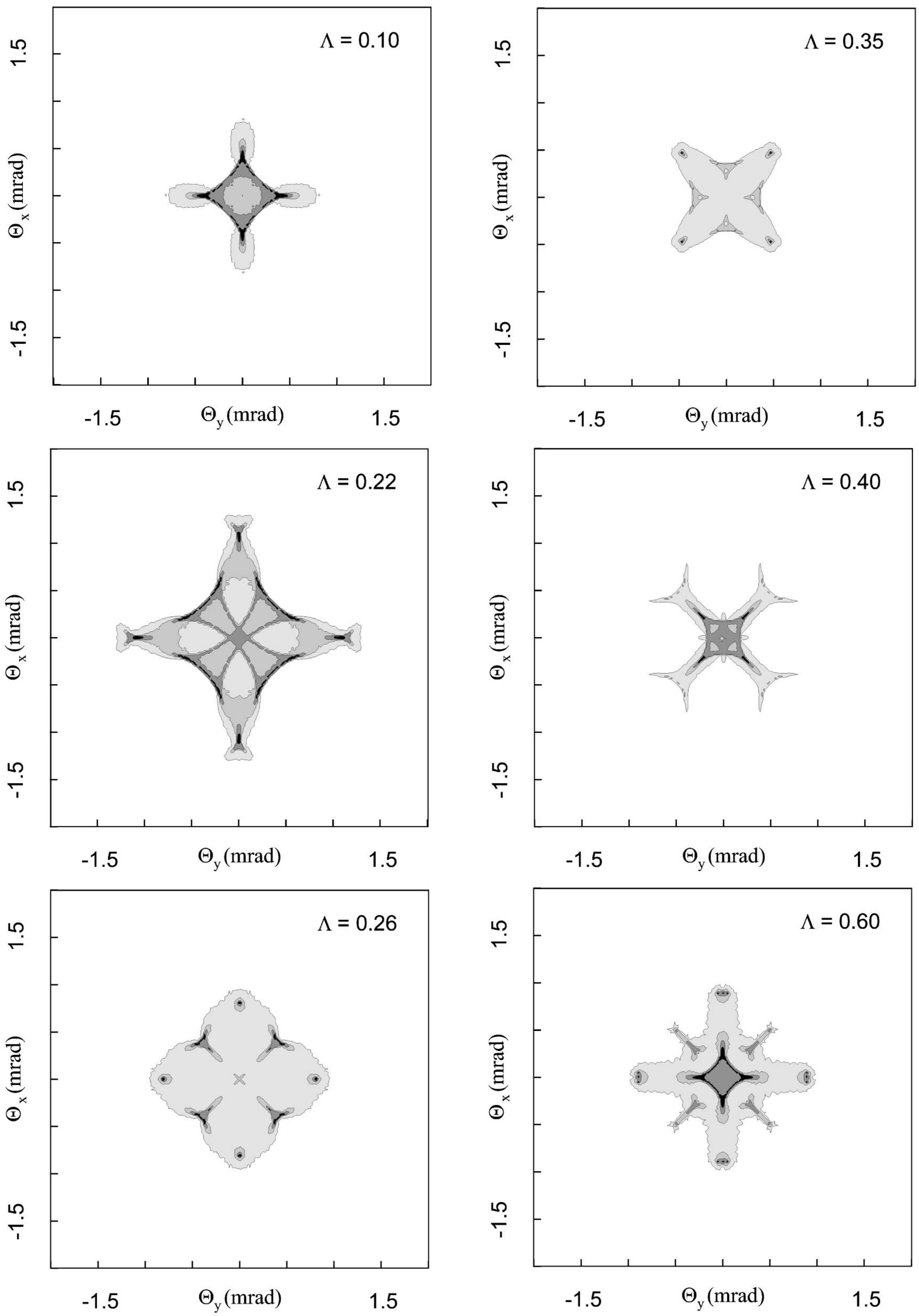


FIG. 1. The angular distributions of $Ne^{10+}$ ions transmitted through a ⟨100⟩ Si thin crystal. The ion energy is 60 MeV and the crystal thicknesses are 105, 232, 274, 369, 422, and 632 atomic layers, corresponding to the reduced crystal thicknesses of 0.10, 0.22, 0.26, 0.35, 0.40, and 0.60. The areas in which the yields of the transmitted ions are larger than 5, 15, 30, and 60% of the maximal yield are designated by the increasing tones of gray color.

number of atomic strings is 36, i.e., we take into account the atomic strings lying on the three nearest (relative to the channel axis) square coordination lines.[17] The average frequency of the transverse motion of the ions is determined from the second-order terms of the Taylor expansion of the continuum potential of the crystal in the vicinity of the channel axis. The equations of motion of the ion in the transverse plane are solved numerically. The components of the impact parameter

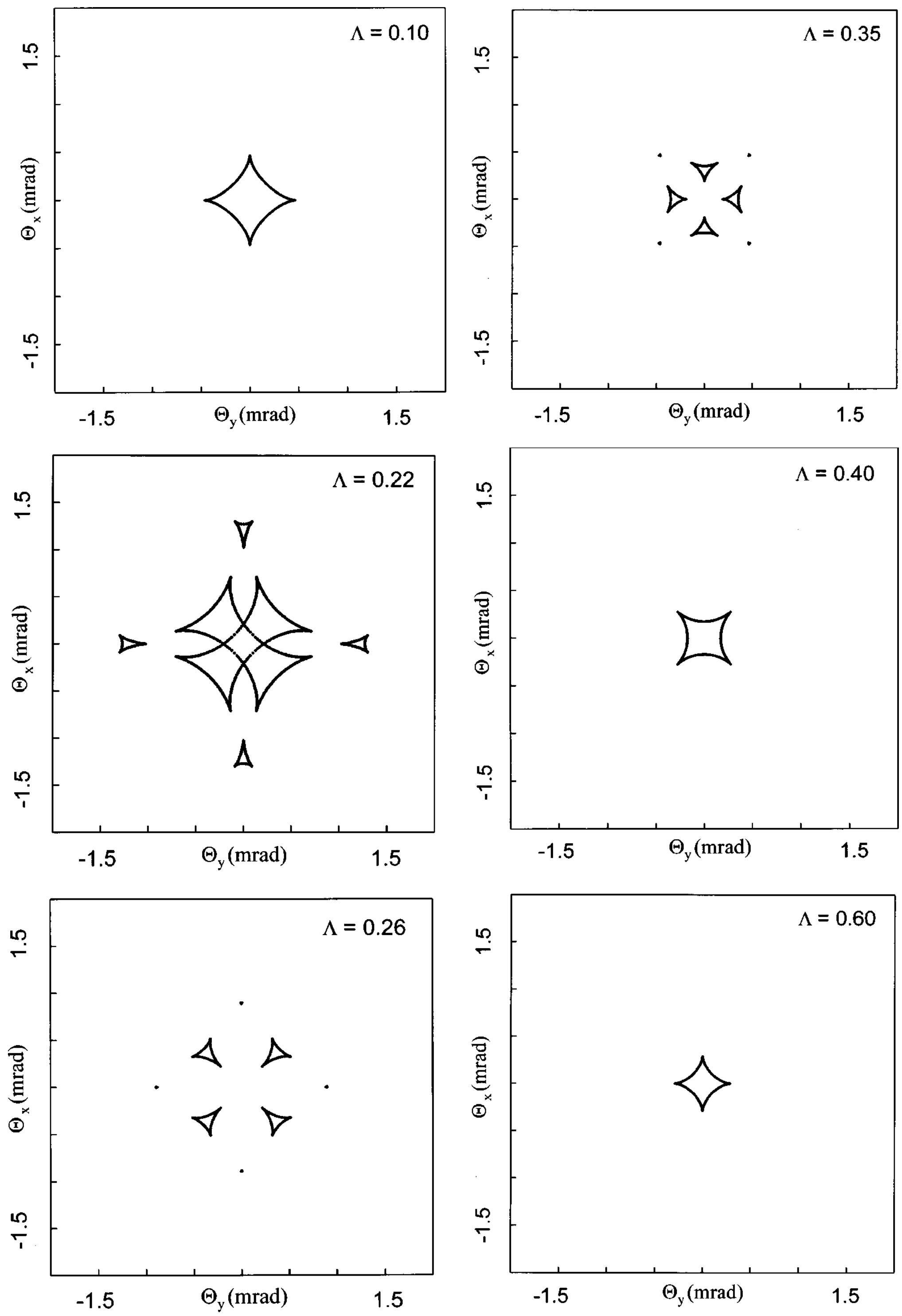


FIG. 2. The rainbow lines in the scattering angle plane for the transmission of $Ne^{10+}$ ions through a ⟨100⟩ Si thin crystal. The ion energy is 60 MeV and the crystal thicknesses are 105, 232, 274, 369, 422, and 632 atomic layers, corresponding to the reduced crystal thicknesses of 0.10, 0.22, 0.26, 0.35, 0.40, and 0.60.

of the ion were chosen uniformly within the region of the channel. The initial number of ions was $709^2 = 502\,681$. The Jacobian of the components of the scattering angle of the ion, and the rainbow lines in the impact parameter plane and scattering angle plane are determined numerically too.

Figure 1 shows the angular distributions of the transmitted ions for the six characteristic values of the reduced crystal thickness—0.10, 0.22, 0.26, 0.35, 0.40, and 0.60. The areas in which the yields of the transmitted ions are larger than 5, 15, 30, and 60 % of the maximal yield are designated by the increasing tones of gray color. The first five values of variable $\Lambda$ correspond to the first rainbow cycle, while its sixth value corresponds to the beginning of the second rainbow cycle. The angular distribution for $\Lambda = 0.10$ is characterized

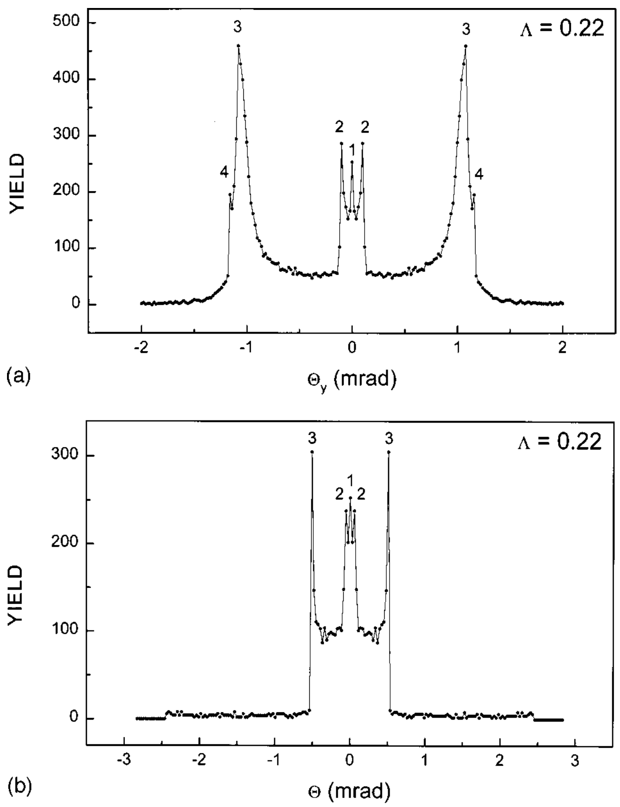


FIG. 3. The yields of $Ne^{10+}$ ions transmitted through a ⟨100⟩ Si thin crystal (a) along the line directed towards the atomic strings defining the channel, and (b) along the line directed between the atomic strings. The ion energy is 60 MeV and the crystal thickness is 232 atomic layers, corresponding to the reduced crystal thickness of 0.22. $\Theta=(\Theta_x{}^2+\Theta_y{}^2)^{1/2}$.

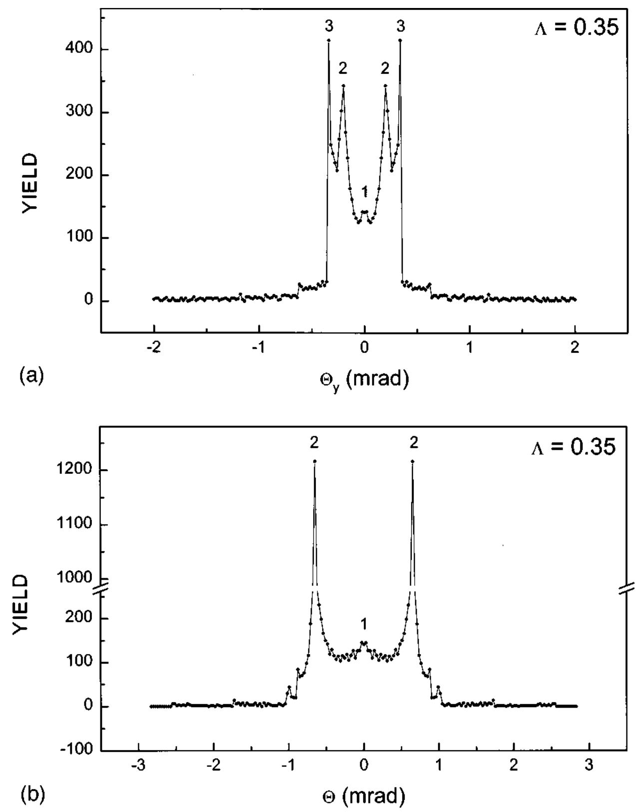


FIG. 4. The yields of $Ne^{10+}$ ions transmitted through a ⟨100⟩ Si thin crystal (a) along the line directed towards the atomic strings defining the channel, and (b) along the line directed between the atomic strings. The ion energy is 60 MeV and the crystal thickness is 369 atomic layers, corresponding to the reduced crystal thickness of 0.35. $\Theta=(\Theta_x{}^2+\Theta_y{}^2)^{1/2}$.

by four pronounced maxima lying on the lines directed towards the atomic strings defining the channel. For $\Lambda=0.22$ and 0.26 the angular distributions contain four pronounced maxima lying on the lines directed towards the atomic strings, and eight pronounced maxima close to the lines directed between the atomic strings. The angular distributions for $\Lambda=0.35$ and 0.40 are characterized by four pronounced maxima lying on the lines directed between the atomic strings. Finally, for $\Lambda=0.60$ the angular distribution is similar to the one for $\Lambda=0.10$, demonstrating the periodicity of the angular distribution with respect to the reduced crystal thickness.

Figure 2 gives the rainbow lines in the scattering angle plane for the six characteristic values of the reduced crystal thickness, as in Fig. 1. The figure includes only the rainbow lines connecting the pronounced maxima of the angular distributions of the transmitted ions. For variable $\Lambda$ equal to 0.10 the rainbow is a cusped square with the cusps directed towards the atomic strings defining the channel. For $\Lambda=0.22$ there are two cusped rectangular rainbows lying along the lines directed between the atomic strings, and four cusped isosceles triangular rainbows along the lines directed towards the atomic strings. For $\Lambda=0.26$ and 0.35 there are four cusped isosceles triangular rainbow lines, and four rainbow points. However, in the former case the rainbow lines lie along the lines directed between the atomic strings, and the rainbow points on the lines directed towards the atomic strings, while in the latter case the arrangement of the rainbow lines and rainbow points is opposite. For $\Lambda=0.40$ the rainbow is a cusped square with the cusps directed between rather than towards the atomic strings. Finally, for $\Lambda=0.60$ the rainbow is again a cusped square with the cusps directed towards the atomic strings. It should be noted that for $\Lambda=0.10$ the rainbow line coincides with the one which would be obtained by the model introduced by Nešković.[12]

The comparison of Figs. 1 and 2 clearly shows that all the pronounced maxima of the angular distributions of the transmitted ions lie on the rainbow lines, i.e., their origin is the crystal rainbow effect. Therefore, we can say that the evolution of the angular distribution with the reduced crystal thickness is fully determined by the evolution of the crystal rainbow.

Figure 3(a) gives the yield of the transmitted ions along the line directed towards the atomic string defining the channel for the reduced crystal thickness equal to 0.22. The comparison of this figure and Fig. 2 shows that the maximum designated by 1 corresponds to the effect of zero-degree focusing of the channeled ions, and the maxima designated by 2, 3, and 4 correspond to the crystal rainbow effect. Maxima 2 correspond to the intersections of the two cusped rectangular rainbows with the $\Theta_y$ axis, while maxima 3 and 4 correspond to the intersections of the two cusped isosceles triangular rainbows with this axis. Figure 3(b) gives the yield of the transmitted ions along the line directed between the atomic strings for variable $\Lambda$ equal to 0.22. Maximum 1 corresponds to the effect of zero-degree focusing, while maxima 2 and 3 correspond to the intersections of the two cusped rectangular rainbows with the $\Theta_x = \Theta_y$ axis.

Figure 4(a) gives the yield of the transmitted ions along the line directed towards the atomic strings defining the channel for the reduced crystal thickness equal to 0.35. The comparison of this figure and Fig. 2 shows that the maximum designated by 1 corresponds to the effect of zero-degree focusing of the channeled ions, and the maxima designated by 2 and 3 correspond to the crystal rainbow effect—to the intersections of the two cusped isosceles triangular rainbow lines with the $\Theta_y$ axis. Figure 4(b) gives the yield of the transmitted ions along the line directed between the atomic strings for variable $\Lambda$ equal to 0.35. The maximum designated by 1 corresponds to the effect of zero-degree focusing, while the maxima designated by 2 correspond to the crystal rainbow effect—to the rainbow points lying on the $\Theta_x = \Theta_y$ axis.

It must be noted that in an experiment the widths of the maxima of the yields of the transmitted ions shown in Figs. 3 and 4 would be larger—primarily due to the uncertainty of the scattering angle of the ion caused by its collisions with the electrons of the crystal, and the finiteness of the resolution of its detector. In order to observe these maxima one must perform a high-resolution experiment similar to the one performed by Krause *et al.*[4]

## IV. CONCLUSIONS

We have presented here the theory of the crystal rainbow. It enables one to generate and fully explain the angular distributions of ions transmitted through thin crystals. The components of the scattering angle of the ion are obtained after solving its equations of motion in the transverse plane, or after the three-dimensional following of its trajectory. The angular distribution is generated by the computer simulation method. Then, the obtained mapping of the impact parameter plane to the scattering angle plane is analyzed, and the rainbow lines in the scattering angle plane are determined. These lines ensure the full explanation of the angular distribution.

The theory of the crystal rainbow has been applied here to the transmission of 60 MeV $Ne^{10+}$ ions through the $\langle 100 \rangle$ axial channels of the Si crystal of the thickness from 105 to 632 atomic layers, i.e., from the beginning of the first rainbow cycle to the beginning of the second rainbow cycle.

This work is the continuation of the experimental and theoretical work of Krause *et al.*,[4,13] which was inspired by the theoretical work of Nešković.[12] We have shown that the evolution of the angular distribution of the transmitted ions with the reduced crystal thickness can be fully explained by the evolution of the crystal rainbow. This means that the theory of crystal rainbow is the proper theory of ion channeling in thin crystals.


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