Eur. Phys. J. B **18**, 553–558 (2000)

THE EUROPEAN PHYSICAL JOURNAL B

EDP Sciences

Rainbows with a ⟨111⟩ Si thin crystal

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Received 11 May 2000

Abstract. This study is devoted to the transmission of Ne^{10+} ions through a ⟨111⟩ Si thin crystal. The ion energy is 60 MeV and the crystal thickness is varied from 159 to 478 atomic layers, *i.e.* within the first rainbow cycle. The analysis is performed by the theory of crystal rainbows. 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.

PACS. 61.85.+p Channeling phenomena (blocking, energy loss, etc.) – 02.40.-k Geometry, differential geometry, and topology

1 Introduction

Axial ion channeling is the motion of ions along axial crystal channels. An axial channel is the part of the crystal in between its neighboring atomic strings. The possibility for such a motion was discovered in a computer simulation of Robinson and Oen [1]. The process can happen if the angle between the initial ion velocity vector and the channel axis is small. The motion of the ion along the channel is explained by a series of its correlated collisions with the atoms of one atomic string resulting in the repulsion of the ion from the string towards the other strings defining the channel. During the process the angle between the ion velocity vector and the channel axis remains small. An analogous explanation is valid for planar ion channeling, in which the ions move along planar crystal channels. A planar channel is the part of the crystal in between its two neighboring atomic planes.

Soon after the discovery of axial ion channeling Lindhard formulated the analytical description of the process [2]. His approach was *via* the formalism of statistical mechanics. The theory includes the continuum approximation, *i.e.* it does not include the (longitudinal) correlations between the positions of the atoms of one atomic string of the crystal. Also, it does not include the (transverse) correlations between the positions of the atomic strings. Besides, it includes the assumption of statistical equilibrium in the transverse plane. In the case of planar ion channeling the theory includes only the analogues of the first and third approximations.

The numerical description of axial ion channeling was formulated by Barrett [3]. His approach was *via* the ion-atom scattering formalism. The theory is applied *via* a very realistic computer code for the three-dimensional following of ion trajectories in channels, in which the three approximations used by Lindhard are avoided. In the case of planar ion channeling the theory is applied in the same way as in the case of axial channeling. The Barrett's approach is more complex, but a number of calculations have shown that it is much more accurate than the Lindhard's one.

We are interested here in the case of axial ion channeling in which the ions are transmitted through the crystal. It is well known that the transverse motion of a channeled ion can be treated as the oscillatory motion around the channel center. If the impact parameter of the ion and the angle between its initial velocity vector and the channel axis are fixed, the number of oscillations the ion makes, before leaving the crystal, depends on its initial energy. If the initial energy of the ion is sufficiently high for it to make, before leaving the crystal, less than about a quarter of an oscillation around the channel center, the ion trajectory can be approximated by a straight line. If this is true for the majority of the ions, we say that the crystal is very thin. If, however, the majority of the ions make, before leaving the crystal, between about a quarter and a few oscillations, we say that the crystal is thin. The crystal is thick, if the majority of the ions make, before leaving the crystal, more than a few oscillations.

It was shown theoretically that in the transmission of ions through axial channels of a very thin crystal the rainbows occurred, *i.e.* in that case the differential transmission cross section of the ion could be singular [4]. The approach of the author was *via* the ion-molecule scattering formalism and it was numerical. In the model 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.

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The crystal rainbow effect was observed for the first time by Krause *et al.* [5].

It was also demonstrated that the crystal rainbows could be classified by catastrophe theory [6–8]. The authors showed that the double cusp catastrophe gives all possible shapes of the rainbow lines in the scattering angle plane in the cases of square, rectangular, centered rectangular and hexagonal very thin crystals with one atomic string per channel. As a result, they obtained a universal, simple and accurate approximation to the continuum potential of the crystal.

Krause *et al.* [9] and Miletić *et al.* [10–12] showed that the evolution of the angular distribution of ions transmitted through a thin crystal with the reduced crystal thickness had a periodic behavior. The study of Krause *et al.* was the report on a high resolution channeling experiment combined with a very accurate calculation using the Barrett's computer code [3]. The reduced crystal thickness is defined by expression $\Lambda = f(Q, m)\, L/V_0$, where Q, m and V_0 are the ion charge, ion mass and initial ion velocity, L is the crystal thickness, and $f(Q, m)$ is the frequency of the transverse motion of the ions moving close to the channel axis. The values of variable Λ equal to 0, 0.5, 1, ... correspond to the beginnings of the cycles of the angular distribution [9]. These cycles are called the rainbow cycles [10]. We can now say that the crystal is very thin, if Λ is smaller than about 0.25, *i.e.* if it comprises less than about a half of the first rainbow cycle.

Petrović *et al.* [13] formulated recently the theory of crystal rainbows, as the generalization of the above mentioned model [4]. They applied the theory to the transmission of Ne^{10+} ions through a ⟨100⟩ Si thin crystal. The ion energy was 60 MeV and the crystal thickness was varied within the first rainbow cycle. They found that the evolution of the angular distribution of the transmitted ions with the reduced crystal thickness could be fully explained by the evolution of the crystal rainbow pattern. It was a clear presentation of the theory of crystal rainbows as the proper theory of ion channeling in thin crystals.

We shall analyze here the transmission of Ne^{10+} ions through a ⟨111⟩ Si thin crystal. The ion energy will be 60 MeV and the crystal thickness will be varied from 159 to 478 atomic layers, *i.e.* within the first 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 pattern.

2 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 [2]. 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 [13].

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

$$V(r) = (Z_1 Z_2 e^2/r)[0.35\exp(-br) + 0.55\exp(-4br) + 0.10\exp(-20br)], \quad (1)$$

where Z_1 and Z_2 are the atomic numbers of the ion and the atoms of the crystal, respectively, e is the elementary charge, 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 [9]. We also assume that we can apply the continuum approximation [2]. The continuum potential of the crystal is the sum of the continuum potentials of its atomic strings.

We shall include here the thermal vibrations of the atoms of the crystal [13]. However, we shall neglect 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 [13].

In order to obtain the components of the scattering angle of the ion, Θ_x and Θ_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 vector. The angular distribution of the transmitted ions is generated by the computer simulation method [4,5,13]. 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.

The scattering law of the ion is given by expressions

$$\Theta_x = \Theta_x(x_0, y_0; \Lambda) \quad \text{and} \quad \Theta_y(x_0, y_0; \Lambda), \quad (2)$$

where x_0 and y_0 are the components of the impact parameter of the ion [13].

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

$$\sigma = 1/|J|, \quad (3)$$

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 [4,5,13].

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

$$J(x_0, y_0; \Lambda) = 0. \quad (4)$$

The rainbow lines in the scattering angle plane are determined by equations (4) and (2), *i.e.* they are the images of the rainbow lines in the impact parameter plane, defined by the scattering law of the ion. These lines separate the bright regions of the scattering angle plane from its dark regions.

3 Results and discussion

We shall analyze here the angular distributions of Ne^{10+} ions transmitted through a ⟨111⟩ Si thin crystal. The ion

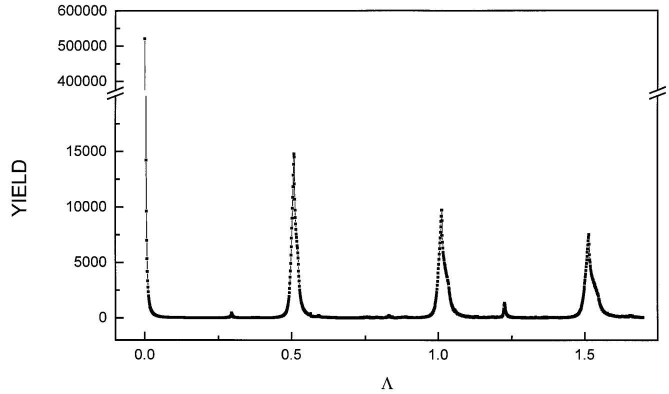

Fig. 1. The dependence of the zero-degree yield of Ne^{10+} ions transmitted through a ⟨111⟩ Si thin crystal on the reduced crystal thickness. The ion energy is 60 MeV.

energy will be 60 MeV and the crystal thickness will be varied from 159 to 478 atomic layers; the thickness of one atomic layer is 0.587904 nm [14]. This range corresponds to the range of the reduced crystal thickness from 0.15 to 0.45, *i.e.* within the first rainbow cycle. The one-dimensional thermal vibration amplitude of the atoms of the crystal is 0.00744 nm [15]. The thin crystal under consideration is a hexagonal one with one atomic string of the crystal per channel [7]. The channel comprises two equilateral triangular subchannels. We assume that the atomic strings defining the channel lie on the x and y axes, and that the subchannel axes lie on the x axis. In order to obtain the proper symmetry of the angular distributions of the transmitted ions and to minimize the computation time, we treat the subchannels as two separate channels and perform the calculations only for the subchannel whose axis lies on the positive part of the x axis [7]. The number of atomic strings is 36, *i.e.* we take into account the atomic strings lying on the three nearest (relative to the subchannel axis) triangular coordination lines. The frequency of the transverse motion of the ions moving close to the subchannel axis is determined from the second order terms of the Taylor expansion of the continuum potential of the crystal in the vicinity of the subchannel center. The equations of motion of the ion in the transverse plane are solved numerically. The components of the impact parameter of the ion are chosen uniformly within the region of the subchannel. The initial number of ions is 260 240. The contribution of the subchannel whose axis lies on the negative part of the x axis is obtained using the fact that the channel is symmetric relative to the y axis. 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 dependence of the yield of the transmitted ions in the region of the scattering angle plane in the vicinity of the origin, *i.e.* the zero-degree yield of the transmitted ions, on the reduced crystal thickness in the range which comprises the first, second and third rainbow cycles. For the region in the scattering angle plane in the vicinity of the origin we took the region in which variable $\Theta = (\Theta_x^2 + \Theta_y^2)^{1/2}$ is smaller than 3×10^{-3} mrad. It is seen clearly that the effect of zero-degree focusing of the transmitted ions exists. The effect is periodic and decays with the reduced crystal thickness [9–12].

Figure 2 shows the angular distributions of the transmitted ions for the six characteristic values of the reduced crystal thickness within the first rainbow cycle – 0.15, 0.20, 0.25, 0.30, 0.34 and 0.45. The corresponding values of the crystal thickness are 159, 213, 266, 319, 361 and 478 atomic layers. The areas in which the yields of the transmitted ions are larger than 7, 15, 35 and 60% of the maximal yield are designated by the increasing tones of grey color. The angular distribution for variable Λ equal to 0.15 is characterized by a hexagonal ridge with six pronounced maxima lying on the lines $\Phi = \tan^{-1}(\Theta_y/\Theta_x) = (2n+1)\pi/6$, $n = 0{-}5$, and six pronounced maxima lying on the lines $\Phi = n\pi/3$, $n = 0{-}5$. For $\Lambda = 0.20$ there is a hexagonal ridge and six pronounced maxima corresponding to the ridge and the pronounced maxima appearing for $\Lambda = 0.15$, and additional six pronounced maxima lying on the lines $\Phi = n\pi/3$, $n = 0{-}5$, in the peripheral region of the scattering angle plane. The angular distribution for $\Lambda = 0.25$ is characterized by a pronounced hexagonal ridge and six pairs of pronounced maxima lying close to the lines $\Phi = n\pi/3$, $n = 0{-}5$. For $\Lambda = 0.30$ there is a maximum lying at the origin, six pronounced maxima lying on the lines $\Phi = n\pi/3$, $n = 0{-}5$, and six pairs of pronounced maxima lying close to these lines. The angular distribution for $\Lambda = 0.34$ is characterized by six pronounced maxima lying on the lines $\Phi = n\pi/3$, $n = 0{-}5$. Finally, for $\Lambda = 0.45$ the angular distribution is similar to the one appearing for $\Lambda = 0.30$.

Figure 3 gives the rainbow lines in the scattering angle plane for the same six characteristic values of the reduced crystal thickness within the first rainbow cycle as in Figure 2.

The figure includes only the rainbow lines connecting the pronounced maxima of the angular distributions of the transmitted ions. For variable Λ equal to 0.15 there are two cusped equilateral triangular rainbow lines with the cusps lying along the lines $\Phi = 2n\pi/3$ and $\Phi = (2n+1)\pi/3$, $n = 0{-}2$. The rainbow pattern for $\Lambda = 0.20$ contains two cusped triangular lines corresponding to the ones appearing for $\Lambda = 0.15$ and a cusped equilateral hexagonal line with the cusps lying along the lines $\Phi = n\pi/3$, $n = 0{-}5$. For $\Lambda = 0.25$ there are three cusped rectangular rainbow lines with the sides perpendicular to the lines $\Phi = 3n\pi/6$, $\Phi = (3n+2)\pi/6$ and $\Phi = (3n+4)\pi/6$, $n = 0{-}3$. The rainbow pattern for $\Lambda = 0.30$ contains six cusped isosceles triangular lines lying along the lines $\Phi = n\pi/3$, $n = 0{-}5$. For $\Lambda = 0.34$ there are six rainbow points lying on the lines $\Phi = n\pi/3$, $n = 0{-}5$. Finally, the rainbow pattern for $\Lambda = 0.45$ contains six cusped isosceles triangular lines similar to the ones appearing for $\Lambda = 0.30$.

The comparison of Figures 2 and 3 clearly shows that all the pronounced maxima of the angular distributions of the transmitted ions, except the maxima lying at the origin, lie on the rainbow lines, *i.e.* their origin is the crystal

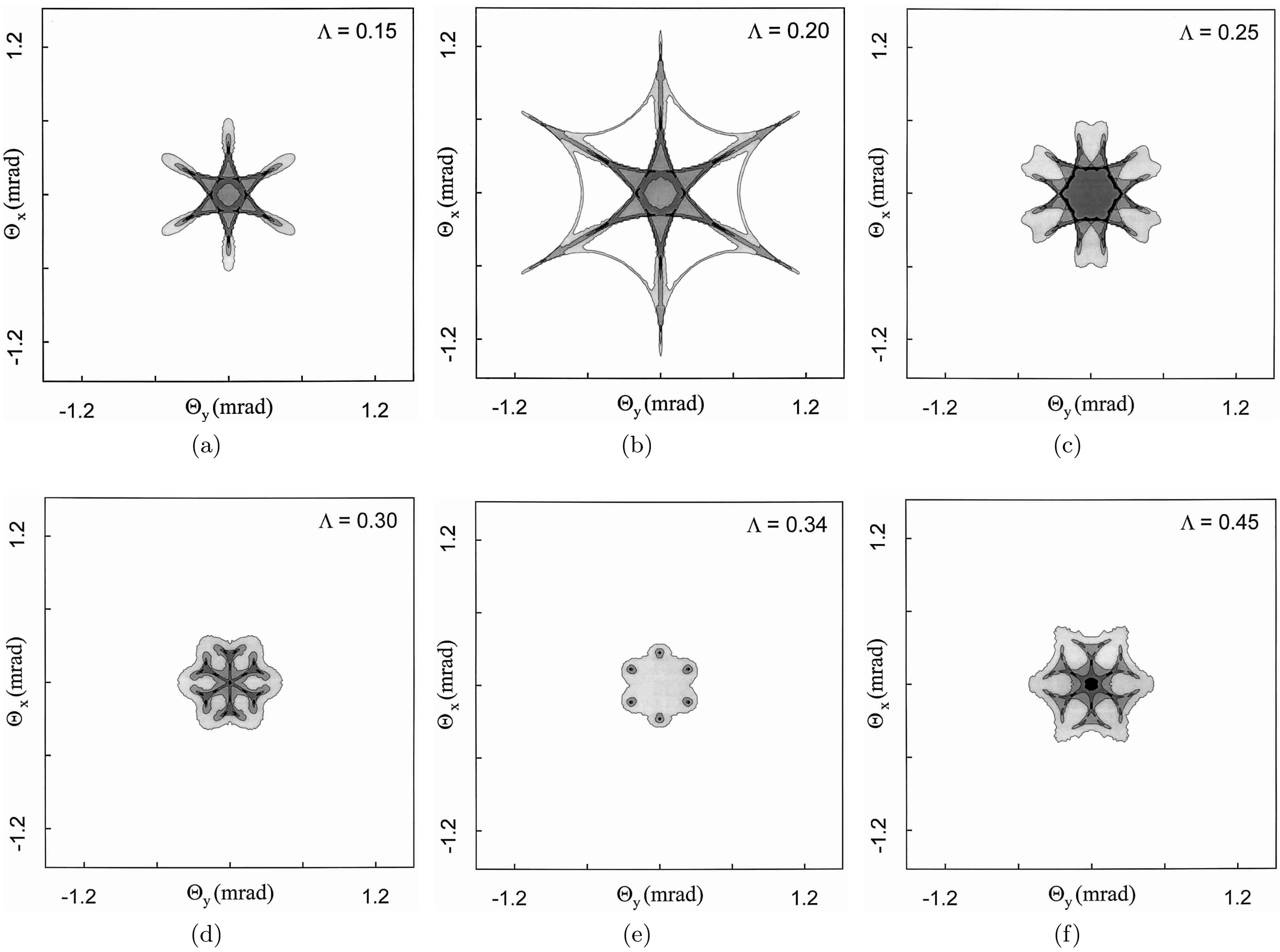

Fig. 2. The angular distributions of Ne^{10+} ions transmitted through a ⟨111⟩ Si thin crystal. The ion energy is 60 MeV and the reduced crystal thicknesses are 0.15, 0.20, 0.25, 0.30, 0.34 and 0.45. The areas in which the yields of the transmitted ions are larger than 7, 15, 35, and 60% of the maximal yield are designated by the increasing tones of grey color.

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 pattern.

Figure 4 gives the yield of the transmitted ions along the Θ_x axis for the reduced crystal thickness equal to 0.20. The comparison of this figure and Figure 3 shows that the maximum designated by 1 corresponds to the effect of zero-degree focusing of the transmitted ions, and the maxima designated by 2, 3 and 4 correspond to the crystal rainbow effect. Maxima 2 correspond to the midpoints between the cusps of the equilateral triangular rainbows, maxima 3 correspond to the apices of the cusps of these rainbows while maxima 4 correspond to the apices of the cusps of the equilateral hexagonal rainbow.

Figure 5 gives the yield of the transmitted ions along the Θ_x axis for the reduced crystal thickness equal to 0.30. The comparison of this figure and Figure 3 shows that the maximum designated by 1 corresponds to the effect of zero-degree focusing of the transmitted ions, and the maxima designated by 2 and 3 correspond to the crystal rainbow effect. Maxima 2 correspond to the apices of the cusps of the first and fourth isosceles triangular rainbows while maxima 3 correspond to the midpoints between the cusps of these rainbows.

It must be noted that in an experiment the widths of the maxima of the yields of the transmitted ions shown in Figures 4 and 5 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.* [9].

4 Conclusion

We have applied here the theory of crystal rainbows to the transmission of 60 MeV Ne^{10+} ions through the ⟨111⟩ axial channels of a Si thin crystal with the thickness varied from 159 to 478 atomic layers, *i.e.* within the first rainbow

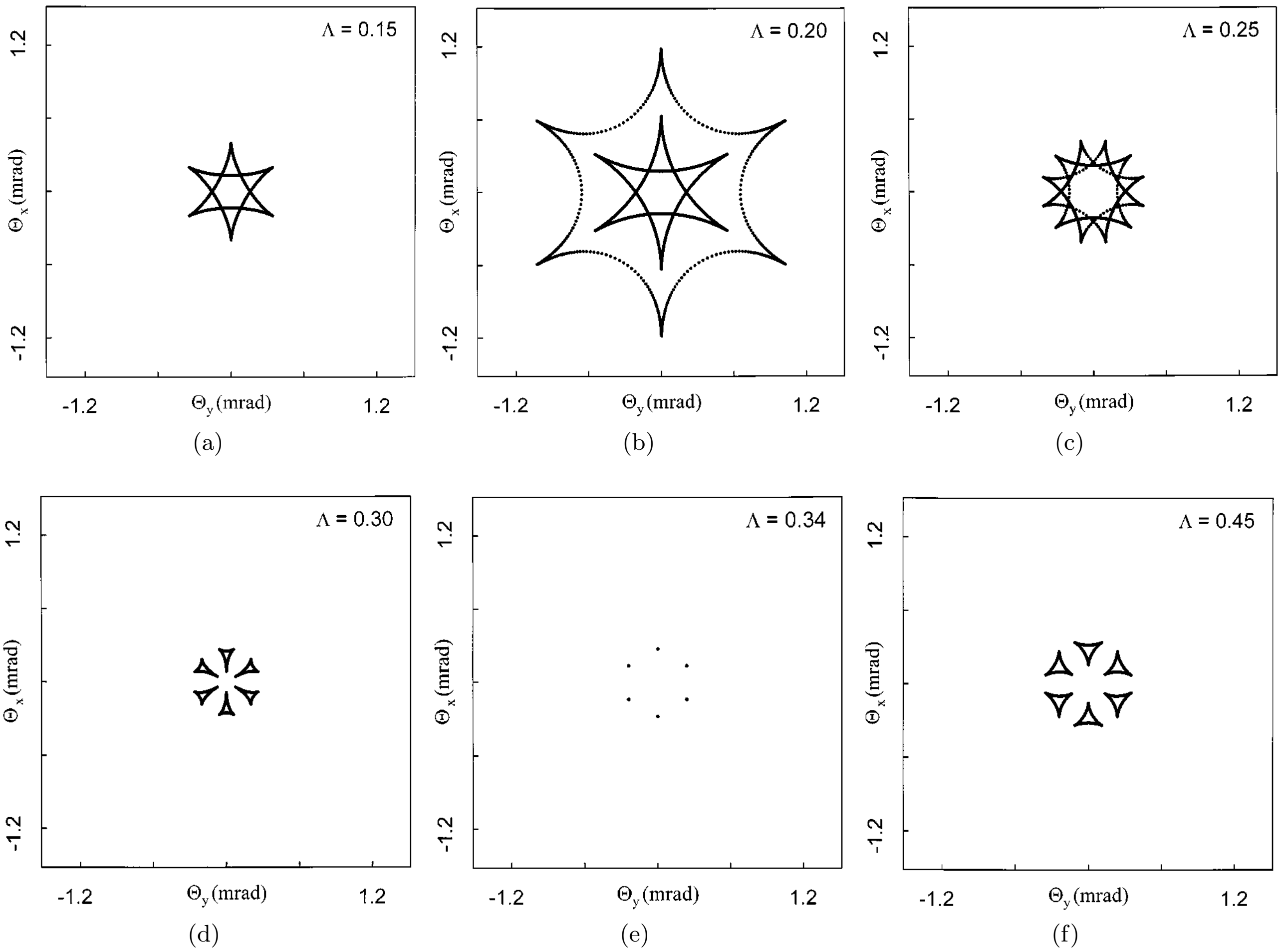

Fig. 3. The rainbow lines in the scattering angle plane for the transmission of Ne^{10+} ions through a ⟨111⟩ Si thin crystal. The ion energy is 60 MeV and the reduced crystal thicknesses are 0.15, 0.20, 0.25, 0.30, 0.34 and 0.45.

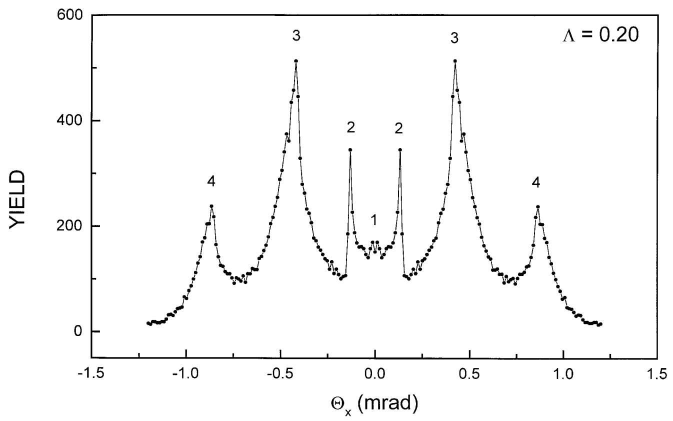

Fig. 4. The yield of Ne^{10+} ions transmitted through a ⟨111⟩ Si thin crystal along the Θ_x axis. The ion energy is 60 MeV and the reduced crystal thickness is 0.20.

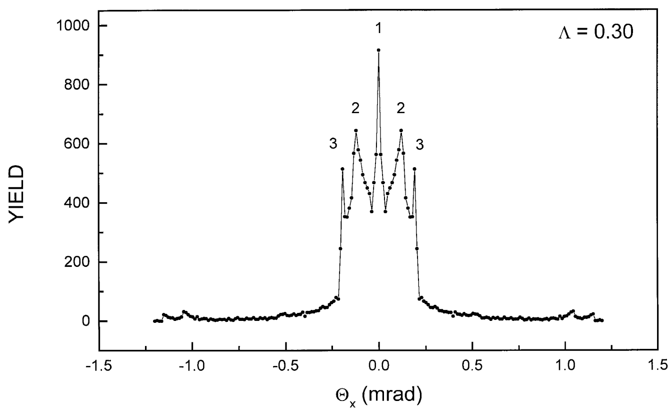

Fig. 5. The yield of Ne^{10+} ions transmitted through a ⟨111⟩ Si thin crystal along the Θ_x axis. The ion energy is 60 MeV and the reduced crystal thickness is 0.30.

cycle. It has been 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 pattern.

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