INFLUENCE OF THE ION BEAM INTERACTION WITH THE CRYSTAL ELECTRONS ON THE ANGULAR DISTRIBUTION OF CHANNELED IONS

by

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This study investigates the effect of crystal electrons on the angular distribution of channeled protons passing through a thin silicon crystal. The effect of crystal electrons on the 2 MeV proton beam channeled through a thin Si crystal plays an important role in the experimentally observed angular distributions. Using the crystal rainbow effect, we have morphologically compared the experimental and theoretical angular distributions of channeled protons and corresponding rainbow lines, with and without the effect of crystal electrons. Our results demonstrate that the influence of crystal electrons affects the angular focus of the channeled ions in the vicinity of the rainbow lines, which are the envelope of this angular distribution. These findings provide insights into the energy loss mechanisms for protons channeled through thin silicon crystals and can have implications for future studies in ion beam physics.

Key words: ion-solid interaction, channeling, crystal rainbow, interaction potential

INTRODUCTION

In recent years, there has been growing interest in the study of ion-solid interactions due to their potential for diverse applications in various fields, such as material science and engineering, and also in microelectronics, nuclear physics, and medical therapy [1, 2]. When an ion beam is incident on a crystalline solid, it interacts with the lattice electrons and nuclei, leading to various phenomena such as radiation damage and ion channeling [2-4]. The channeling process is a phenomenon that takes place when an ion beam is directed towards a single crystal in a direction close to a major crystallographic axis. Under such conditions, the ion will undergo a sequence of correlated grazing collisions with the atoms of the strings forming the crystal channel. As a result, the ion experiences an oscillatory motion as it travels through the spaces between the atomic strings, resulting in a well-defined path within the crystal lattice, see fig. 1.

The energy loss theory attributed to electronic stopping in amorphous media has been widely established, with the Bethe-Bloch equation showing accurate experimental results within a few percent [2]. In amorphous media, after averaging all possible impact

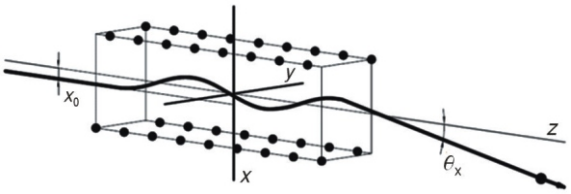

Figure 1. The schematic process of ion transmission through an axial crystal channel

parameters, the local electron density distribution has been also averaged and therefore does not exhibit a distinct effect on the energy loss. However, for ions transmitted through a single crystal, the distribution of ion trajectories is altered due to the channeling effects, highly deviating from its average distribution. As a result, channeled ions' energy loss relies on the distribution of ion trajectories and the local electron density distribution. The phenomenon and theoretical analysis of energy loss for channeled ions become more intricate, as other factors that impact the trajectory or electron distribution can influence the energy loss. This characteristic adds to the fascinating nature of studying energy loss in channeled ions [4].

The dominant process that occurs in channeling is the rainbow channeling effect, whose theory was formulated by Petrović *et al*. [5]. This theory accurately predicts angular distributions of ions channeled

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through crystals. Analogous to the scattering of sunlight from water droplets [6], the crystal rainbow effect divides the angular distribution of transmitted ions into the *bright* and *dark* parts *i. e*., the rainbow lines in the rainbow channeling effect presents an envelope of angular distributions of channeled ions. Furthermore, due to a strong focusing of ions along the rainbow lines they represent a "skeleton" of the angular distribution. As the explanation of the so called "doughnut" effect, that appears when an ion beam is not perfectly aligned with the primary crystallographic axis, the existence of rainbow lines has been proven in a series of high-resolution ion transmission channeling experiments through ultra-thin silicon membranes [7]. Subsequent to these findings, it has been demonstrated that the experimental results and theory underlying the crystal rainbow effect have scientific applications in accurately determining the interaction potential between ions and crystals [8]. In addition, recent research has shown that the crystal rainbow effect can be employed to identify the thermal vibrations and defects of monolayer graphene sheets, which has implications for the development of novel materials and devices [9, 10]. It is also possible to perform a morphological analysis of graph sheets using the crystal rainbow theory [11, 12]. The rainbow channeling effect is so dominant that characteristic spatial rainbows are even observed in the case of transmission of protons through octopole electrostatic lenses, where dimensions of characteristic rainbow patterns are at a macroscopic scale [13-15]. The various applications of the rainbow channeling demonstrate its usefulness as a precise theory for investigating the process of ion channeling. Recently we managed to construct the universal rainbow channeling interaction potential for 28 crystals with a cubic crystallographic structure via the morphological method [16-18].

THEORY

The motion of an ion transmitted through a crystal channel can be classically described using Newton's equation of motion [5]

$$\frac{\mathrm{d}\,\vec{p}}{\mathrm{d}t} \qquad U_{\mathrm{ch}}(\vec{p}) \tag{1}$$

where $\vec{p}$ is the ion momentum, t – the time, U_{ch} – the continuum ion-crystal interaction potential, and $\vec{p}$ – the transverse vector of ion position relative to the atom of atomic strings defining the crystal channel.

Figure 1 illustrates the process of ion channeling through a (001) channel of a cubic crystal. The reference system has a longitudinal z-axis that aligns with the channel axis, while the vertical and horizontal axes are x and y, respectively. The ion's initial impact parameter is given by $\vec{b} = b(x_0, y_0)$. The interaction between ions and crystals is modeled using the continuum approximation and the ion-atom binary collision model [4]. In this framework, the interaction potential between a channeled ion and the atomic strings that define the crystal channel reads [3, 4]

$$U_i(\rho_i) \quad \frac{1}{d} \int_{-\infty}^{\infty} V[(\rho_i^2 \quad z^2)]^{1/2}\mathrm{d}\,z \tag{2}$$

where $U_i(\rho_i)$ represents the continuum interaction potential between the ion and the i^{th} atomic string, d – the distance between neighboring atoms within the atomic string, $\rho_i^2 = (x - x_i)^2 + (y - y_i)^2$ is the distance between the ion and the i^{th} atomic string, and x and y are the transverse components of the particle position vector, x_i and y_i are the coordinates of the i_{th} atomic string. The ion-atom interaction potential is denoted by V. The continuum ion-crystal interaction potential, U_{ch}, is the sum of the continuum potentials of all atomic strings U_i taken into account. In addition, the model incorporates the effects of thermal vibrations of the crystal atoms [5].

The theory behind rainbow channeling is based on an analysis of the mapping of the impact parameter (IP) plane to the transmission scattering angle (SA) plane, which is determined by the channeling/transmission process [5]. The obtained mapping is given by

$$\theta_x \quad \theta_x(x_0, y_0) \text{ and } \theta_y \quad \theta_y(x_0, y_0) \tag{3}$$

where θ_x and θ_y are components of the transverse exit ion channeling angle.

The IP SA mapping, defined by the functions (3), depends on fixed parameters such as the ion energy, crystal channel, and thickness. To obtain this mapping, one must solve the ion equations of motion and determine its exit angle. Uniform initial positions are selected for the ion in the entrance plane of the crystal, and the initial ion velocity vector v_z is parallel to the z-axis. It is worth noting that the channeled ion angle with respect to a channel axis is always smaller than the critical angle for channeling [3, 4], and in this case the transverse exit angles are: $\theta_x = v_x/v$ and $\theta_y = v_y/v$; the transverse components of the exit ion velocity are denoted by v_x and v_y, respectively.

As the components of the ion scattering angle remain small throughout the channeling process, the differential transmission cross-section for the exit ions corresponding to an impact parameter can be expressed as follows [5]

$$\sigma(x_0, y_0; \theta_x, \theta_y) \quad \frac{1}{\left|J_\theta(x_0, y_0)\right|} \tag{4}$$

where $J_\theta(x_0, y_0) = x_0\,\theta_x \quad y_0 \quad _y - y_0\,\theta_x \quad x_0 \quad _y$ is the Jacobian of the mapping (3).

Therefore, the equation

$$J_\theta(x_0, y_0) \quad 0 \tag{5}$$

defines the rainbow lines in the impact parameter plane. Along these lines the σ is infinite. The rainbow lines in the SA plane, which are the images of the mapping of the rainbow lines determined by function (5), separate bright and dark regions of the angular distribution of channeled ions. These lines represent the singularities of the corresponding mappings from the IP plane to the SA plane. Thus, the rainbow effect is an example of a singularity effect.

We applied the expression for the electronic energy loss of the ion to calculate the energy loss of the channeled protons [19]

$$\frac{\mathrm{d}E}{\mathrm{d}x} \quad \frac{4\pi Z_1^2 e^4}{m_e v^2} n_e \ln \frac{2m_e v^2}{\hbar \omega_e} \tag{6}$$

where

$$\omega_e \quad \frac{4\pi e^2}{m_e} n_e \quad ^{1/2} \tag{7}$$

and

$$n_e \quad \frac{1}{4\pi Z_1 e^2} \sum_{i\ 1}^{M} (\partial_{xx} \quad \partial_{yy}) V_i^{th} \tag{8}$$

The atomic number of the ion is denoted by Z_1, v is the incident ion velocity, the electron mass is m_e, and ω_e – the angular frequency of the oscillations of the electron gas of the crystal induced by the ion, average density of the electron gas is n_e, which varies with the ion's position in the transverse plane (x, y), V_i^{th} denotes the thermally averaged continuum interaction potential of the ion and the ith atomic string [19] and the number of atomic strings taken into account is M. Equation (6) represents the well-known Bethe formula, which is commonly used to calculate the electronic energy loss of high energy charged particles in matter.

Scattering angle uncertainty caused by the ion-electron collisions within the crystal is taken into account via the following formula [20],

$$\frac{\mathrm{d}\ _e^2}{\mathrm{d}z} \quad \frac{m_e}{2m_i E} \quad \frac{\mathrm{d}E}{\mathrm{d}z} \tag{9}$$

$_e$ is the mean square angular deviation and m_i – the ion mass. Our study has been focused on the influence of the ion scattering with the crystal's electrons on the angular distributions of 2 MeV H^+ ion beams oriented along the three major crystallographic axes in a Si crystal. We used numerical solutions of the ion's equations of motion and computer simulation methods to determine the angular distributions of channeled ions. The fourth-order Runge-Kutta method [21] was utilized for the simulations. To ensure a random distribution of ions within the crystal channel, we uniformly distributed the ion's initial positions in the transverse plane.

Our morphological method involves comparing the rainbow lines in the SA plane with the experimental and theoretical angular distributions of channeled 2 MeV protons passing through thin silicon membranes in all three major crystallographic orientations, both with and without the effect of scattering with the crystal's electrons. This method can improve our understanding of the channeling process and more accurately reproduce the future channeling experimental result. One benefit of this method is that it can lead to more precise measurements of the ion-atom interaction potential.

RESULTS AND DISCUSSION

The effect of the interaction of a channeled ion with crystal electrons is primarily influenced by the local electron density distribution. Therefore, this effect is trajectory dependent. This chapter presents our theoretical results on the angular distribution of channeled 2 MeV protons passing through thin silicon membranes in all three major crystallographic orientations. Our approach utilizes a morphological method that compares the rainbow lines in the SA plane with the experimental [8, 16-18] and theoretical [16-18] angular distributions of channeled ions, both with and without the effect of crystal electrons.

The shape and size of the silicon crystal channel varies depending on its orientation. The (001) orientation has a square-shaped channel defined by a single atomic array per node. The (011) orientation has a rhombus-shaped channel defined by two atomic arrays per node. The (111) orientation has a hexagonal-shaped channel consisting of two sub-channels in the shape of equilateral triangles defined by a single atomic array per node. The thicknesses of the crystals were 55 nm, 29 nm, and 43 nm, for the (001), (011), and (111) orientations, respectively that correspond to approximately 101, 75, and 91 atomic layers. We took into account atomic strings lying on the three nearest symmetrical coordination lines relative to the channel axis, with values of M = 36, 72, and 36, for the (001), (011), and (111) orientations, respectively. The variations in channel shape and size, along with crystal thickness, play a crucial role in determining the angular distribution of channeled ions and the morphology of the rainbow lines, ultimately providing valuable insights into the structural properties of the crystal and the interaction mechanisms between the ions and the crystal atoms. The ion energy was taken to be 2 MeV, and a total of 4 10^6 incident ions were used in the simulations. Circular regions with a radius equal to the screening length around atomic arrays exhibiting strong potential values that can cause significant scattering of fast-moving ions, rendering them unable to follow a path through the crystal lattice. As a result, these regions are not available for channeled ion positions, and their avoidance is necessary for reliable channeling simulations. Using computer simulation methods, we obtained the angular distributions of the transmitted ions by numerically solving the equations of motion of the ion-equations (1). Using the crystal

rainbow theory, we compared the rainbow lines in the scattering angle plane without the effect of the scattering of ions with the crystal's electrons and the ions' angular distributions, taking into account the scattering of ions with the crystal's electrons.

Figure 2 displays the angular distributions of channeled protons through a 55 nm thick silicon crystal oriented along (001), with rainbow lines generated using different interaction potentials, considering both without fig. 2(a) and with the effect of crystal electrons fig. 2(b), respectively. We chose a thickness of 55 nm for a Si crystal oriented along the (001) direction because it has been both experimentally and theoretically established that under these conditions, the angular distributions of 2 MeV channeled protons can be accurately described using crystal rainbow theory [8]. It is worth noting that, to the best of the authors' knowledge, this experimental result represents the only instance in channeling where a sufficiently high resolution has been achieved to enable a meaningful comparison between the angular distributions of transmitted ions and the crystal rainbow lines. Also, in the work presented in ref. [8] the crystal rainbow theory and a morphological method were used to construct the rainbow interaction potential. The angular distributions of channeled protons exhibit a remarkably close agreement with the inner and outer rainbow lines generated using the rainbow interaction potential. Additionally, the inner rainbow lines generated using the Moliere interaction potential align well with the inner angular distributions of channeled protons, while the outer rainbow line generated using the famous Ziegler, Biersack and Littmark interaction potential (ZBL further in text) corresponds favorably with the outer angular distribution. These findings, extensively discussed in refs. [8, 16-18], emphasize that the crystal rainbow theory appropriately explains the channeling effect. Our rainbow interaction potential proves to be an exceptionally precise description of the angular distributions of channeled protons. Comparing fig. 2(a) and 2(b) demonstrates that the proton beam's angular distribution is notably influenced by crystal electrons, particularly in the proximity of the rainbow lines. Figure 2(b) and the discussion in ref. [8] indicate that accounting for crystal electron influence through our numerical model, utilizing the adopted energy loss mechanism aligns the resulting angular distributions of channeled protons with those obtained using the realistic FLUX three-dimensional simulation code [22]. This observation underscores the satisfactory performance of our model.

Figure 3 presents the angular distributions of 2 MeV protons channeled through a 29 nm thick silicon crystal in the (011) orientation relative to the proton beam and their corresponding rainbow lines. Figure 3(a) showcases the angular distributions without considering the interaction with the crystal's electrons,

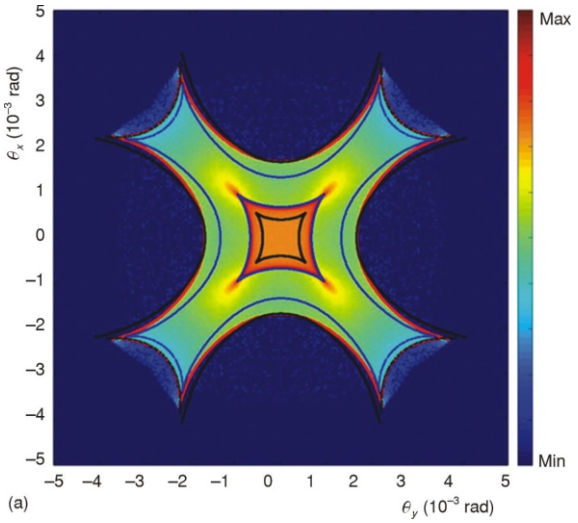

Figure 2(a). Angular distributions of protons transmitted through (001) oriented Si crystal without the effect of crystal electrons, and corresponding rainbow lines (red – Rainbow potential, blue – Moliere potential, black – ZBL potential, in electronic version)

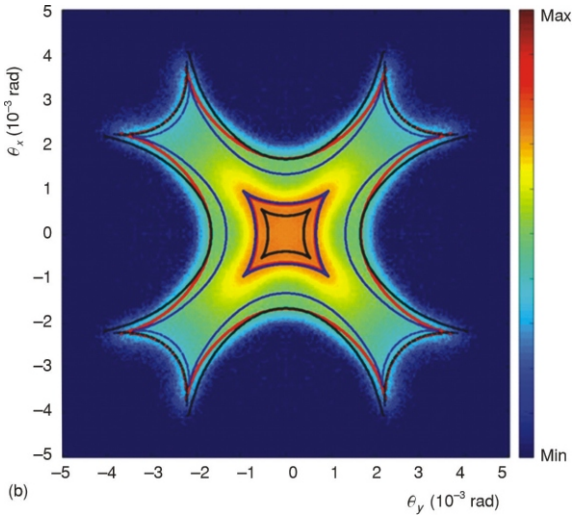

Figure 2(b). Angular distributions of protons transmitted through (001) oriented Si crystal with the effect of crystal electrons, and corresponding rainbow lines (red – Rainbow potential, blue – Moliere potential, black – ZBL potential, in electronic version)

while fig. 3(b) demonstrates the same distribution with the inclusion of the interaction with the crystal's electrons. As already mentioned in a previous case, the corresponding inner and outer rainbow lines are the envelopes of the calculated angular distributions. Since the (011) channel of the Si crystal is one of the largest channels in nature, from fig. 3 and eq. 6, it is clear that the influence of crystal electrons is much more prominent in the outer region of the angular distribution, *i. e*., in the vicinity of the outer rainbow line. Also, it is clear that the channel area in the vicinity of the outer rainbow line, undergoes a considerably more significant influence compared to the area in the vicin-

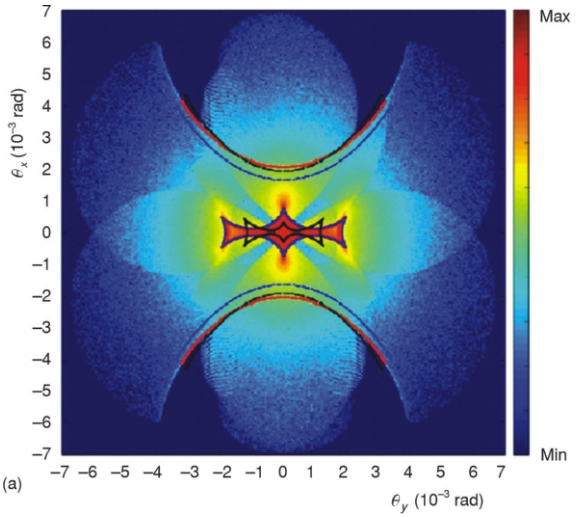

Figure 3(a). Angular distributions of protons transmitted through (110) oriented Si crystal without the effect of crystal electrons, and corresponding rainbow lines (red – Rainbow potential, blue – Moliere potential, black – ZBL potential, in electronic version)

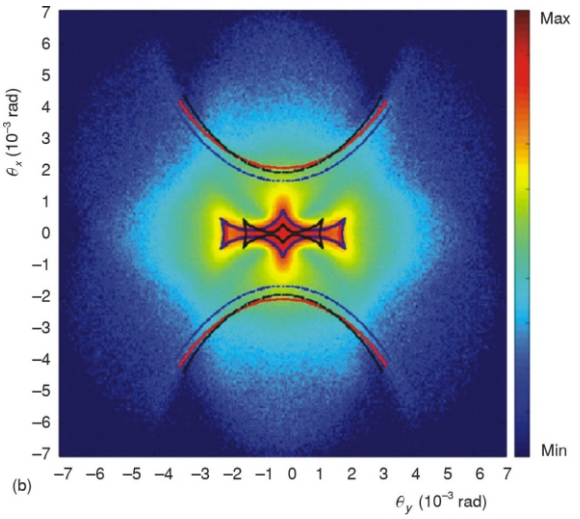

Figure 3(b). Angular distributions of protons transmitted through (110) oriented Si crystal with the effect of crystal electrons, and corresponding rainbow lines (red – Rainbow potential, blue – Moliere potential, black – ZBL potential, in electronic version)

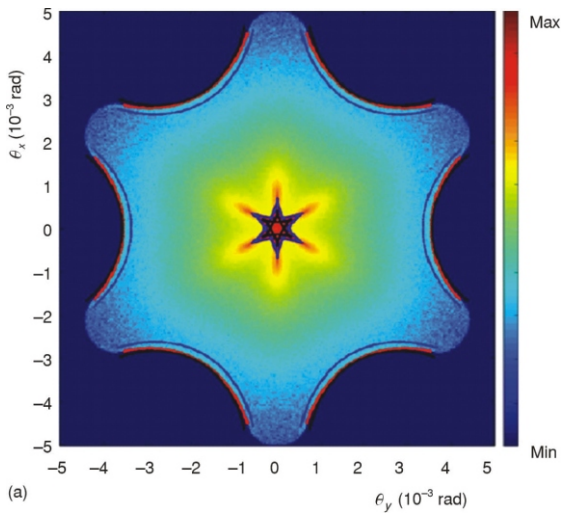

Figure 4(a). Angular distributions of protons transmitted through (111) oriented Si crystal without the effect of crystal electrons, and corresponding rainbow lines (red – Rainbow potential, blue – Moliere potential, black – ZBL potential, in electronic version)

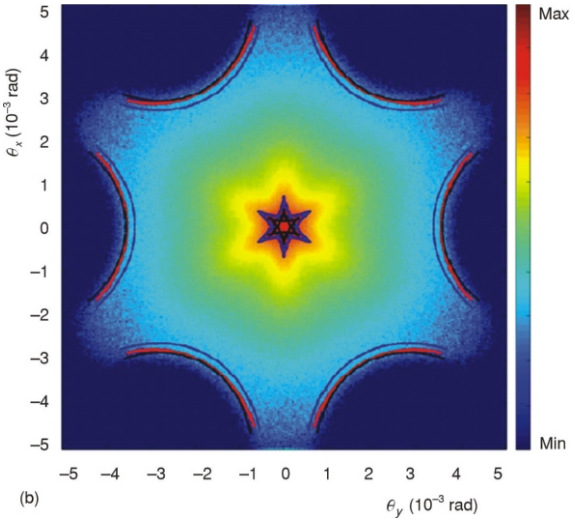

Figure 4(b). Angular distributions of protons transmitted through (111) oriented Si crystal with the effect of crystal electrons, and corresponding rainbow lines (red – Rainbow potential, blue – Moliere potential, black – ZBL potential, in electronic version)

ity of the inner rainbow line. Further, it should be stressed that the difference between the inner rainbow lines generated by the ZBL and the rainbow potential is very pronounced showing an excellent case for the experimental test of the validity of the rainbow potential.

Figure 4 shows the angular distributions of 2 MeV protons channeled through a 43 nm thick silicon crystal in the (111) orientation relative to the proton beam and their corresponding rainbow lines. Figure 4(a) displays the angular distributions without considering the interaction with the crystal's electrons, while fig. 4(b) shows the identical distributions with the inclusion of the interaction with the crystal's electrons. As mentioned earlier, the morphology of proton angular distributions and the shape of their corresponding rainbow lines are primarily determined by the positions of atomic strings defining the crystal channel rather than the overall shape of the channel. Consequently, even though the (011) and (111) orientations share the same rhombus-shaped channel, the distinct arrangements of atomic strings in these orientations lead to a clear difference in angular distributions of channeled protons and the positions and shapes of the rainbow lines. This distinction highlights the sensitivity of the channel's geometry to the precise positions of atomic strings, ultimately shaping the scattering behavior and accounting for the observed differences in the angular distributions. In the case of the (111) orientation of the Si crystal, which has a much

smaller channel compared to the (001) and (011) orientations, the influence of electrons on the angular distributions is strong throughout the entire area of the crystal channel. This means that both the inner and the outer rainbow lines are similarly influenced.

One can see that the outer rainbow line forms a cusped hexagon shape with its corners truncated by the atomic screening radius. On the other hand, the inner rainbow line is composed of two rainbow lines in the shape of cusped equilateral triangles, which are a consequence of two sub-channels. Due to the small size of the (111) Si channel, the influence of crystal electrons on the broadening of proton angular distributions is significant and the angular distribution appears to lack its fine structure along rainbow lines. However, the distinct outer and inner fine structure in the shape of a six-pointed star which matches the outer and inner rainbow line, is observable in fig. 4(b).

CONCLUSION

In this article, we employed the morphological method to investigate the angular distribution of channeled ions through thin Si crystals in all three major crystallographic orientations. The investigation focused on understanding the influence of the effect of the crystal electrons on the angular distributions of transmitted protons. The influence of the crystal electrons and its connection with the energy loss effect was adopted from reference [4]. Crystal rainbow theory was utilized to compare rainbow lines with theoretically obtained distributions of 2 MeV protons transmitted through thin Si crystals oriented along (001), (011), and (111) crystallographic directions. In all three crystal orientations, the influence of the crystal's electrons resulted in observable changes in the angular distributions of transmitted protons, particularly in the vicinity of the rainbow lines. It should be noted here that the (011) and (001) orientation are in that sense more favorable for the (experimental) analysis of the inner structure, while the (001) and (111) for the outer structure of the angular distribution. This conclusion leads to an interesting possibility of connecting the electron energy loss via the effect of the interaction with the crystal's electrons. This method can contribute to advancing experimental studies in channeling by providing a means to reproduce and interpret future experimental results accurately, thus enhancing our understanding of the phenomenon.

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AUTHORS' CONTRIBUTIONS

All authors contributed to the study's conception and design. N. S. Starčević and S. M. Petrović performed material preparation, data collection, and analysis. N. S. Starčević wrote the first draft of the manuscript, and all authors provided feedback and made revisions to previous versions of the manuscript. All authors have read and approved the final manuscript.

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УТИЦАЈ ИНТЕРАКЦИЈЕ ЈОНСКОГ СНОПА СА ЕЛЕКТРОНИМА КРИСТАЛА НА УГАОНУ РАСПОДЕЛУ КАНАЛИСАНИХ ЈОНА

Ова студија истражује ефекат електрона кристала на угаону расподелу протона каналисаних кроз танки кристал силицијума. Утицај електрона кристала на сноп каналисаних протона енергије 2 MeV кроз танак кристал Si игра важну улогу у експериментално добијеним угаоним расподелама. Користећи ефекат кристалне дуге, морфолошки смо упоредили експерименталне и теоријске угаоне дистрибуције каналисаних протона и одговарајућих линија дуге, са и без утицаја електрона кристала. Наши резултати показују да утицај електрона кристала утиче на угаони фокус каналисаних јона у околини линија дуге, које представљају скелет угаоне расподеле. Ови резултати пружају увид у механизме енергијских губитка протона каналисаних кроз танки кристал силицијума и могу имати импликације за будуће студије у физици јонског снопа.

Кључне речи: интеракција јона и чврстог тела, каналисање, кристална дуга, потенцијал интеракције