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Angular dependence for the energy loss of channeled He ions near the Si⟨1 1 0⟩ and ⟨1 1 1⟩ directions

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Abstract

In the present work, we report on measurements of angular dependent energy loss for 1.2 and 2.0 MeV He ions incident near the Si ⟨1 1 0⟩ and ⟨1 1 1⟩ axes parallel to the {1 0 0} and {1 1 0} planes, respectively. The measurements were done using the Rutherford backscattering technique (RBS) combined with a SIMOX sample. The experimental results are well reproduced by calculations based on the convolution approximation for the impact-parameter dependence of the energy loss of the core electrons. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

The energy transferred in an inelastic collision of an energetic ion with an atom, at a given impact parameter, is an essential quantity in the study of the slowing-down process of charged particles in crystals. When an ion beam penetrates into an amorphous solid, the distribution of the impact parameters of the ions with respect to the target electrons is uniform. However, if the target is a monocrystalline material, and the beam impinges on the crystal parallel to a low index axial direction, the situation becomes quite different. A sizeable fraction of beam particles is under the conditions of best channeling, moving in the central part of the channel, undergoing, however, small transverse oscillations. In this situation, the ions stopping power can be drastically reduced, as compared to the one along a non-aligned direction [1,2]. This feature can be explained through the impact-parameter dependence of the energy loss in an ion–atom collision. Since well-channeled ions maintain large impact parameters with respect to the atom rows, they can only transfer very small amounts of energy to the inner shell electrons of the target. In addition, the contribution of valence electrons to the stopping may also be reduced, due to their low density in the center of the channel.

The transverse space allowed for channeled particles depends on their so-called transverse energy. Tilting the axis channel relatively to the

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beam, brings as a consequence the increase of the transverse energy, modifying the ion flux distribution across the channel, so that smaller impact parameters are sampled by the particles. Therefore, by measuring the angular dependence of the stopping power for channeled ions, detailed information can be inferred on the impact-parameter dependence of the inelastic energy loss. Despite the importance of this kind of study, few results have been reported in the literature, and most of them deal with protons and He in Si single crystals [3–8]. Only recently, results for the angular dependent energy loss of Li channeled near the $\langle 1\,0\,0\rangle$ direction have been published [9].

From the theoretical point of view, a full analysis of the stopping of channeled ions is not a trivial task. It requires a precise knowledge of (a) the ion flux distribution across the channel and (b) the electronic energy loss as a function of the impact parameter for different charge states of the projectile. On the other hand, the theoretical treatment of the energy loss has evolved over the time. From semi-empirical models [10], it developed into first-order [11] and full calculations, such as the coupled-channel method [12–14], the last ones being very much computer time-consuming. Very recently, Grande and Schiwietz [15] have developed a first principle calculation method which allows the determination of the energy loss $Q(b)$ as a function of the impact parameter b. The method, called perturbative convolution approximation (PCA), was later improved, giving rise to the unitary convolution approximation (UCA) [16]. Therefore, taking into account the UCA method together with the calculated flux distribution of the ions along the channel, it is possible to determine the energy loss as a function of the impact parameter, from first principle calculations, and without a heavy computational work.

In order to investigate the dependence of the energy loss on the impact parameter, we undertook the present work, where we have measured the channeling energy-loss for He ions as a function of a Si single crystal orientation. At variance with most of the studies dealing with angular dependence of the energy loss, which have been done via the transmission geometry [3–6], this work was carried out by using the backscattering technique (RBS) together with a SIMOX target. Though, unlike our previous publications [7,8], where we have explored the $\langle 1\,0\,0\rangle$ axial direction, in the present case, we investigate the He energy loss along the Si $\langle 1\,1\,0\rangle$ and $\langle 1\,1\,1\rangle$ axes parallel to the $\{1\,0\,0\}$ and $\{1\,1\,0\}$ planes, respectively. In addition, from the theoretical standpoint, while in [4–6] and [7] the experimental results were discussed in terms of the semi-classical approximation (SCA) [11] and coupled-channel method [12–14], respectively, this is the first time that the UCA model [16] is used to describe the angular dependence of the channeling stopping power.

2. Experimental procedure

In the present experiment, we have used the RBS technique together with a SIMOX target, as described in detail in [7]. In summary, the SIMOX sample used in the present experiment consisted of a 200 nm Si$\langle 1\,0\,0\rangle$ crystal layer on top of a 500 nm SiO_2 buried layer produced in a Si$\langle 1\,0\,0\rangle$ wafer. The sample was prepared at the IBM T.J. Watson Research Center, New York, and, as revealed by transmission electron microscopy, the upper Si/SiO_2 interface was sharp (less than 2 nm of roughness) and did not show any significant level of extended defects. Before each experiment, the sample was cleaned and etched using 10% HF to remove the native surface oxide film and other impurities sitting on the surface. Afterwards, the sample was mounted on a three-axis goniometer with 0.005° precision, and, immediately after, the chamber was evacuated reaching a final vacuum of 10^{-7} Torr.

The He beam was produced by the 3 MV Tandetron at the Physics Institute of the *Universidade Federal do Rio Grande do Sul*, in Porto Alegre (Brazil). The divergence of the He beam was less than 0.03° full width. The backscattered particles were detected by a Si surface barrier detector placed at 170° with respect to the beam direction. The overall detector and electronic resolution of the system was about 13 keV full width at half-maximum.

The measurements were taken with respect to the Si$\langle 1\,1\,0\rangle$ and $\langle 1\,1\,1\rangle$ axes parallel to the $\{1\,0\,0\}$

and {1 1 0} planes, respectively. The scans around the ⟨1 1 0⟩ axis were performed at 1.2 and 2 MeV, whereas the beam energy was 1.2 MeV, for the ⟨1 1 1⟩ direction. After determining the channeling direction ($\Psi = 0°$), we have recorded RBS spectra, for different values of the angle of incidence, Ψ, ranging between $-2°$ and 2°, in 0.2° steps. Due to the crystallographic orientation (⟨1 0 0⟩) of the SIMOX sample employed in the present study, we were not able to accomplish an azimuthal average of the energy loss values.

Typical RBS/channeling spectra taken with 2 MeV He beam at angles $\Psi = 0°$, 0.4°, 0.5° and 0.6° with respect to the ⟨1 1 0⟩ direction are shown in Fig. 1. The spectrum for non-aligned directions are also displayed. The spectrum for well-channeled particles show two basic features: (a) the minimum backscattering yield, χ_{min}, corresponding to the near surface region is $\chi_{min} = 3\%$, while the one corresponding to the upper Si/SiO_2 interface is $\chi_{min} = 5\%$; (b) the Si/SiO_2 interface is – taking into account the straggling in the Si film – as sharp as the front Si edge. These features show, on the one hand, that the Si crystal film is of very good quality and, on the other, that the Si/SiO_2 interface is very well defined, as also indicated by the TEM observations provided by the supplier.

3. Data analysis and experimental results

The energy loss was obtained by fitting the spectra with an algorithm which takes into account the fact that the backscattering yield, at a given detected energy, is due to two components: (a) the one that corresponds to those particles which are truly backscattered inside the channel; and (b) the one that is due to those which are first dechanneled (most likely into a random direction) and then backscattered. As the incident angle increases, the latter contribution to the RBS spectrum becomes quite substantial, so that a simple analysis based only in the determination of the edge position of the upper Si/SiO_2 interface does

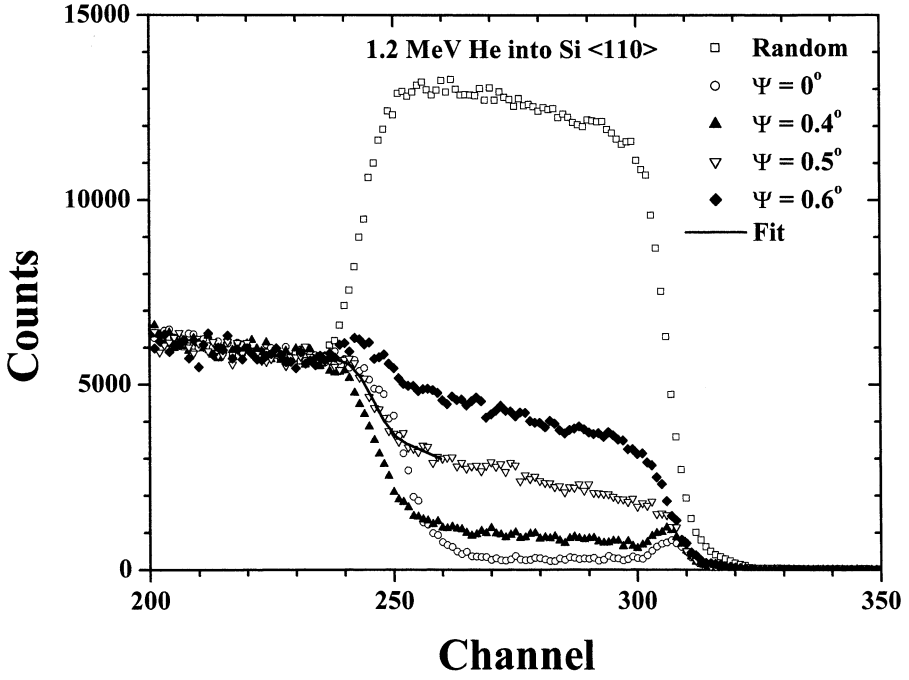

Fig. 1. Random and channeling RBS spectra of a SIMOX target taken with a 2 MeV $^4He^{2+}$ beam incident at $\Psi = 0°$, 0.4°, 0.5° and 0.6° with respect to the ⟨1 1 0⟩ axis parallel to the {1 0 0} plane.

not provide accurate results and can even be misleading. In the above-mentioned algorithm, it is assumed that the channeled fraction of the beam decreases exponentially with the depth. For further details on the data treatment, the reader is referred to [7]. The solid line in Fig. 1 shows the result of the fitting procedure applied to a RBS/channeling spectrum.

The α ratio between the channeling and the random (taken from [17]) stopping power as a function of the angle of incidence, Ψ, of He ions impinging near the $\langle 1\,1\,0\rangle$ and $\langle 1\,1\,1\rangle$ directions of Si is shown in Fig. 2. An important feature seen in Fig. 2(a) is that the width of the $\alpha(\Psi)$ curve is about half of the width of the *minimum yield*, $\chi_{\min}$, versus Ψ curve. This means that there are channeling trajectories where He ions probe an energy loss rate as large as along a non-aligned direction. Finally, one can see from Fig. 2 that, in some cases, the α ratio reaches values above unity, which implies that the stopping power of channeled ions under certain conditions can exceed the random one. This issue shall be addressed in Section 5.

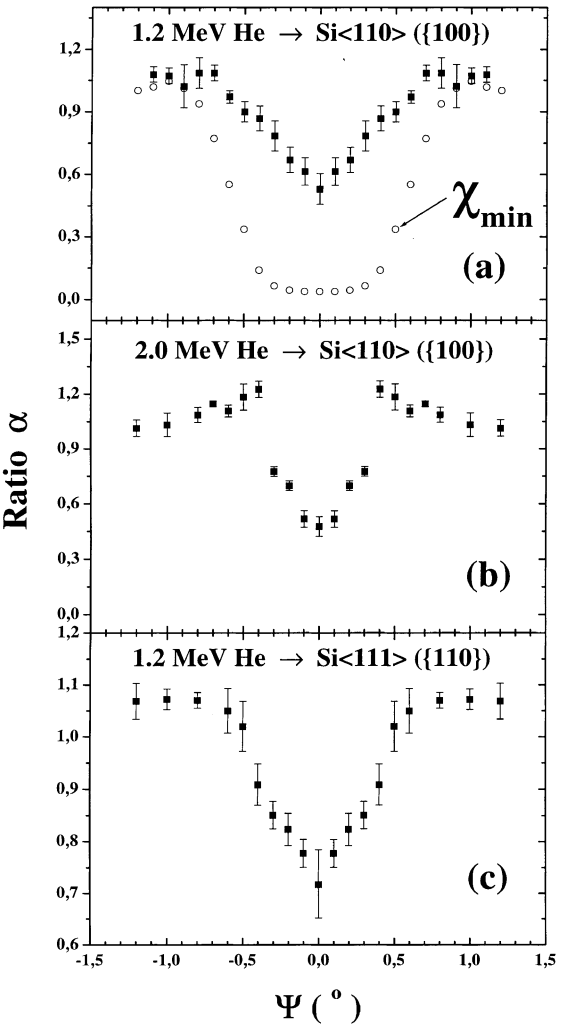

Fig. 2. Ratio between channeling and random stopping powers of He ions as a function of the angle of incidence relative to the $\langle 1\,1\,0\rangle$ (at 1.2 MeV (a) and 2.0 MeV (b)) and $\langle 1\,1\,1\rangle$ (c) (at 1.2 MeV) axes.

4. Theoretical procedure

The sequence of correlated collisions undergone by the beam particles, under the condition of axial channeling, focus the beam in the central region of the channel (flux peaking). This effect explains the reduced channeling stopping power in comparison with the random one. When the angle of incidence of the beam increases, the particles flux inside the channel tends to become uniform. However, the channeling stopping power depends not only on the ion flux, but also on the inelastic energy Q transferred in a binary collision at impact parameter b. The average energy lost by the beam, ΔE, after traversing a thickness t of the crystal, can be calculated through the following equation:

$$\Delta E(\Psi, E_0) = \frac{1}{d}\frac{\int_A d^2\rho\Phi(E_0,\Psi,\vec{\rho})Q_{\text{total}}(\vec{\rho},E_0)}{\int_A d^2\rho\Phi(E_0,\Psi,\vec{\rho})}, \quad (1)$$

where E_0 is the incident beam energy, d the interatomic distance along the channel axis, A the transverse area of the channel, $\vec{\rho}$ the transverse distance of the element of area $d^2\rho$ with respect to the center of channel, and $\Phi(E_0,\Psi,\vec{\rho})$ is the flux through the area element $d^2\rho$ averaged along the thickness t. $Q_{\text{total}}(\vec{\rho},E_0)$ is the energy transferred by an ion passing across the channel, at the position $\vec{\rho}$.

In order to calculate the energy lost by a channeled ion as a function of its transverse position, $Q_{\text{total}}(\vec{\rho})$, we have to take into account the

contribution of each of the n Si atoms around the axis channel, so that

$$Q_{\text{total}}(\vec{\rho}) = \sum_{i}^{n} Q(b_i). \tag{2}$$

Eq. (1) relates a macroscopic quantity, namely the energy loss as a function of incidence angle, with a microscopic one, $Q(b)$, which contains the interaction between the projectile and the electronic system of the target atom. The quantity that makes this connection is the ion flux distribution.

4.1. Calculation of the ion flux through the channel

In order to obtain the ion flux through an element of area $d^2\rho$, we have to determine, from an *ensemble* of trajectories, the ones that effectively pass through the area element $d^2\rho$, at a depth between z and $z + dz$. The channeling trajectories were calculated in the continuum approximation [18], using the ZBL potential [19] for a row of atoms. The thermal vibration of the crystal atoms was taken into account by the convolution between the potential of a static row of atoms and a Gaussian distribution for the transverse displacements of these atoms with respect to their equilibrium positions. The vibrational amplitude used was of 0.083 Å, according to the Debye temperature of [20].

The potential $U(x, y)$, which governs the transverse motion of channeled particles, was obtained by adding the potential of the first neighbor rows of atoms. The number of rows considered was seven for the $\langle 1\,1\,1\rangle$ axis, and six for the $\langle 1\,1\,0\rangle$ one. We have tried larger number of atoms rows in the calculation of $U(x, y)$, but it did not modify the results of the simulation. For each incident ion followed in the simulation, the impinging position on the channel transverse surface was chosen in a random way, whereas the transverse component of its initial velocity is determined by the angle of incidence of the beam. Then the ion trajectories were determined by numerically solving the Newton's equations of motion for the potential $U(x, y)$.

4.2. Determination of the impact-parameter dependent energy-loss

Schiwietz and Grande [16] proposed a very simple model to calculate $Q(b)$, which not only gives the same results of first-order calculations for all impact parameter values, but also takes into account non-perturbative effects to the energy loss, with no need of a heavy computational work. The authors have shown that, in first-order, $Q(b)$ is essentially the convolution of the target electronic density with a certain *kernel*. In this model, called UCA, the sum of the transition probabilities is normalized to unity through the constraint that the stopping cross-section equals the value given by the Bloch theory. The model was implemented in a computer code called convolution approximation for swift particles (CASP). Further details can be found in [16] as well as in the web [21].

When a He beam, at energies above 300 keV, penetrates into a Si target, only two charge states are populated, namely, He^+ and He^{2+} [22]. Therefore, we have to consider only the energy transfers by He^+ and He^{2+} ions, $Q^+(b)$ and $Q^{2+}(b)$, respectively. An He^{2+} ion can excite or ionize the target atoms as well as can capture electrons from the Si atom. Hence, Q^{2+} is given by

$$Q^{2+}(b) = Q^{2+}_{\text{exc}}(b) + Q^{2+}_{\text{cap}}(b), \tag{3}$$

where Q^{2+}_{exc} correspond to ionizations or excitations of the target atom, and Q^{2+}_{cap} is due to electron-capture process.

In turn, an He^+ ion can also produce excitations or ionizations of the target atoms. Additionally, in the He^+ frame of reference, the Si atoms may be regard as projectiles, which can excite or ionize the He^+ ion. Thus,

$$Q^{+}(b) = Q^{+}_{\text{exc}}(b) + Q^{+}_{\text{loss}}(b), \tag{4}$$

where Q^{+}_{loss} is the contribution from process of ionization or excitation of the He^+ ion *by* the Si atom. It is worthwhile to emphasize that the calculations based on the UCA model from the CASP program do not account for the contribution from electron-capture process. However, this contribution should be of minor importance for

well-channeled particles, since He^+ and He^{2+} ions capture mostly from Si inner shell electrons. Then, the average impact-parameter dependent energy-loss is given by the following expression:

$$Q(b) = f_+(Q^+_{\mathrm{exc}}(b) + Q^+_{\mathrm{loss}}(b)) + f_{2+}Q^{2+}_{\mathrm{exc}}(b), \qquad (5)$$

where f_+ and f_{2+} are the equilibrium fraction of ions in the He^+ and He^{2+} charge states, respectively. For the charge states fractions, we took the experimental values of [22]. Finally, it is important to point out that the UCA calculations provide reliable energy loss values, as shown recently in [23,24].

5. Discussion

In Fig. 3, we compare the theoretical results, based on the UCA model, with our experimental results. For 1.2 MeV He ions inciding near the $\langle 1\,1\,1\rangle$ Si direction, the agreement with the experimental results is quite good – see Fig. 3(a). Nevertheless, the calculated $\mathrm{d}E/\mathrm{d}x$ value around $\Psi = 0°$ is slightly underestimated. This discrepancy can be due to the fact that the UCA model does not account for electron-capture or other higher order process, such as the Barkas effect (polarization). Although the electron-capture mechanism plays an essential role in the charge equilibration process, its contribution to the energy loss is of minor importance. On the other hand, the good agreement for larger angles of incidence can be explained by the fact that, under these conditions, an overestimated Q_{exc} should compensate for the lack of capture or polarization in the model [24]. Nevertheless, concerning the $\langle 1\,1\,0\rangle$ direction – Figs. 3(b) and (c) – a remarkable theoretical–experimental agreement can be observed.

In the present work, as mentioned before, the experimental stopping power values were not azimuthally averaged. Instead, the angular scans were taken along planar directions and, consequently, for particular large angles of incidence, we have obtained energy loss values larger than the random one ($\alpha > 1$), as depicted by the "shoulders" of the curves shown in Fig. 2(b). This feature might be

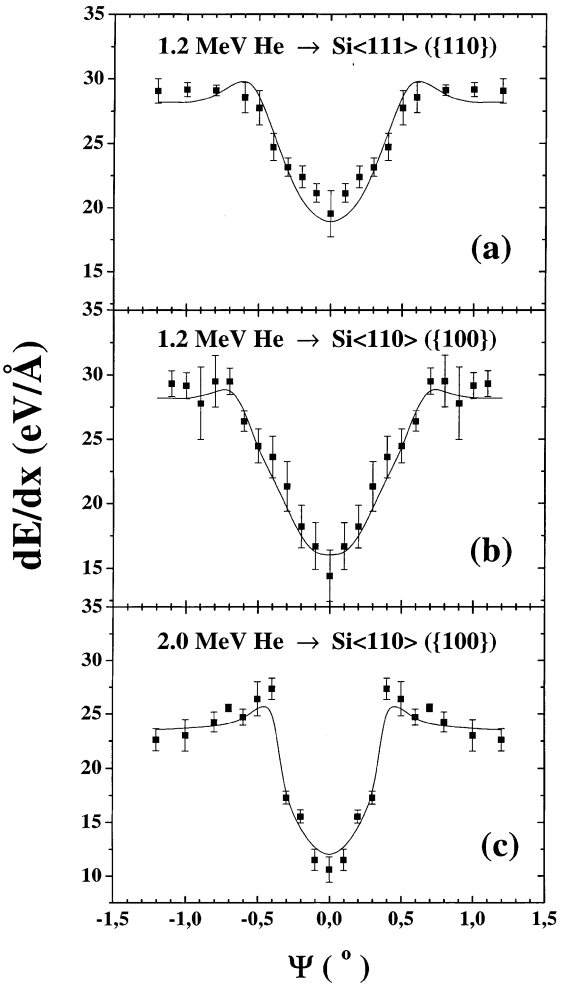

Fig. 3. Comparison between the experimental and theoretical results for the stopping power of He ions as a function of the angle of incidence relative to the $\langle 1\,1\,1\rangle$ (a) and $\langle 1\,1\,0\rangle$ ((b) and (c)) axes.

explained in terms of the ion flux distribution. Indeed, in Fig. 4 is shown the ion flux through the $\langle 1\,1\,0\rangle$ channel as a function of distance for different values of the angle of incidence. As can be observed, for $\Psi = 0.6°$ the ion flux is concentrated near the $\{1\,1\,0\}$ planes, giving rise to energy losses larger than the ones corresponding to non-aligned directions. On the other hand, it should be noted that in our previous works [7–9], the azimuthal average of the energy loss values has systematically produced stopping ratios smaller than 1.

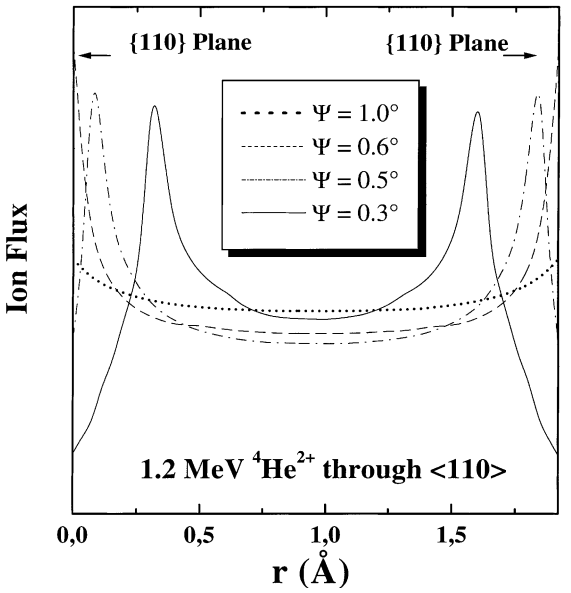

Fig. 4. Flux of channeled He ions along the Si ⟨1 1 0⟩ direction for different angles of incidence.

6. Conclusions

In the present work, we have measured and calculated the energy loss of He ions at 1.2 and 2 MeV as a function of the angle of incidence near the Si ⟨1 1 0⟩ and ⟨1 1 1⟩ axes parallel to the {1 0 0} and {1 1 0} planes, respectively. For this purpose, we have used the RBS combined with a SIMOX target, using the upper Si/SiO_2 interface as a marker.

The theoretical analysis was performed by taking into account the ion flux distribution, the impact parameter dependence of the energy loss, and the charge states of the ions. The ion flux was determined using the continuum potential model taking into account the ZBL potential [19]. The impact-parameter dependence of the energy loss was calculated by using the UCA approximation from the CASP program. This model was developed by Schiwietz and Grande [16] and it is based on the SCA. A comparison between the experimental results and the theoretical calculations shows a remarkable agreement for all the studied cases, independently of the energy or the Si direction under study.

In some cases, for large angles of incidence, the measured channeling energy loss was larger than the random one. This feature might be explained on the basis that, for increasing angles of incidence, the flux tends to concentrate near the atomic planes.

References

[1] D.S. Gemmell, Rev. Mod. Phys. 46 (1974) 129.
[2] D.V. Morgan (Ed.), Channeling: Theory, Observation, and Applications, Wiley, London, 1973.
[3] H.S. Jin, W.M. Gibson, Nucl. Instr. and Meth. B 13 (1986) 76.
[4] A. Dygo, M.A. Boshart, M.W. Grant, L.E. Seiberling, Nucl. Instr. and Meth. B 93 (1994) 117.
[5] A. Dygo, M.A. Boshart, L.E. Seiberling, N.M. Kabachnik, Phys. Rev. A 50 (1994) 4979.
[6] M.A. Boshart, A. Dygo, L.E. Seiberling, Phys. Rev. A 51 (1995) 2637.
[7] J.H.R. dos Santos, P.L. Grande, M. Behar, H. Boudinov, G. Schiwietz, Phys. Rev. B 55 (1997) 4332.
[8] G. de M. Azevedo, M. Behar, J.F. Dias, P.L. Grande, J.H.R. dos Santos, R. Stoll, Chr. Klatt, S. Kalbitzer, Nucl. Instr. and Meth. B 136 (1998) 132.
[9] G. de M. Azevedo, J.F. Dias, J.H.R. dos Santos, P.L. Grande, M. Behar, Chr. Klatt, S. Kalbitzer, Nucl. Instr. and Meth. B 161–163 (2000) 145.
[10] O. Oen, M. Robinson, Nucl. Instr. and Meth. B 132 (1976) 647.
[11] N.M. Kabachnik, V.N. Kondratev, O.V. Chumanova, Phys. Stat. Sol. B 145 (1988) 103.
[12] G. Schiwietz, Phys. Rev. A 42 (1990) 296.
[13] G. Schiwietz, P.L. Grande, Nucl. Instr. and Meth. B 69 (1992) 10.
[14] P.L. Grande, G. Schiwietz, Phys. Rev. A 47 (1993) 1119.
[15] P.L. Grande, G. Schiwietz, Phys. Rev. A 58 (1998) 3796.
[16] G. Schiwietz, P.L. Grande, Nucl. Instr. and Meth. B 153 (1999) 1.
[17] D. Niemann, P. Oberschachtsiek, S. Kalbitzer, H.P. Zeindl, Nucl. Instr. and Meth. B 80–81 (1993) 37.
[18] J. Lindhard, Mat. Fys. Medd. K. Dan. Vidensk. Selsk. 34 (1965) 1.
[19] J.F. Ziegler, J.P. Biersack, U. Littmark, in: J.F. Ziegler (Ed.), The Stopping and Ranges of Ions in Matter, Vol. 1, Pergamon, New York, 1985.
[20] G. de M. Azevedo, J.C. Martini, M. Behar, P.L. Grande, Nucl. Instr. and Meth. B 149 (1999) 301.
[21] http://www.hmi.de/people/Schiwietz/casp.html.
[22] R.J. Petty, G. Dearnaley, Phys. Lett. 50A (1974) 273.
[23] G. de M. Azevedo, P.L. Grande, G. Schiwietz, Nucl. Instr. and Meth. B 164 (2000) 203.
[24] G. de M. Azevedo, D.L. da Silva, J.F. Dias, M. Behar, P.L. Grande, G. Schiwietz, Phys. Rev. B, to be published.