HYPERCHANNELING OF Ne^{10+} IONS THROUGH THE THICK <111> Si CRYSTALS

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Abstract. In this work we investigate the angular distributions of Ne¹⁰⁺ ions hyperchanneled along the <111> direction in a thick silicon crystals as a function of the reduced crystal thickness. The ion energy is 60 MeV and the reduced crystal thickness, Λ , is varied from 10 to 21, corresponding to the crystal length from 6.2 to 13.1 μ m. We follow the ion trajectory in the triangular region of the crystal channel determined by the maximum closed equipotential line around the channel axis, where the hyperchanneling occurs. The Hénon-Heiles type of the ion-crystal interaction potential is used as the model of the continuum interaction potential obtained assuming the Molière expression for the ion-atom interaction potential. The angular distributions are generated using the numerical solution of ion's equations of motion in the transverse plane and the computer simulation method. The obtained results show periodicity of the angular distribution, with the period of 0.5. The values of $\Lambda = 10$, 10.5, 11, ..., 21, correspond to the beginnings of periodic cycles of the angular distribution. The effect of zero-degree focusing is observed for these values of variable Λ . Also, one can observe the formation of the symmetrical ridges in the angular distributions around the centre of the scattering angle plane, whose number increases and the average distance between them decreases as the variable Λ increases.

1. INTRODUCTION

Hyperchannelling effect occurs when motion of the channelled ion is restricted to only one crystal channel (Gemmell 1974). The hyperchanneling region is then determined by the maximum closed equipotential line around the channel axis. In this region electron density is low comparing with the rest of the crystal and one can call hyperchanneling the "pure" channeling since the trajectory of channeled ion is always far away from the atomic strings defining the channel.

In this work we investigate the angular distributions of Ne¹⁰⁺ ions hyperchanneled along the <111> direction in the thick silicon crystals as a function of the reduced crystal thickness. The ion energy is 60 MeV and the reduced crystal thickness, $\Lambda = f \times L/V_0$, where f is the frequency of transverse ion motion close to the channel axis, L is the crystal thickness, and V_0 is initial ion velocity (Krause et al. 1994; Miletić et al. 1996), is varied from 10 to 21, corresponding to the crystal length from 6.2 to 13.1 μ m.

2. THEORY

We consider an ion moving along axial channel in the $\langle 111 \rangle$ direction of a thick silicon crystal. The atomic strings defining the channel lie on the x and y axes, and the negative direction of z axis coincides with the channel axis. The origin lies in the entrance plane of the crystal. The initial ion velocity vector is parallel to the channel axis $\vec{v} = -v\vec{e}_z$. We assume that the interaction of the ion and the crystal is elastic and that it can be treated classically. Also, we assume that we can apply the continuum approximation (Lindhard 1965). For the "exact" continuum interaction potential of the ion and i-th atomic string we use the potential based on the Molière's expression for the ion-atom interaction potential (Petrović et al. 2000; Nešković et al. 2000):

$$U_i(\rho) = \frac{2Z_1 Z_2 e^2}{d} \sum_{i=1}^3 \alpha_i K_0(\beta_i \frac{\rho}{a_s})$$
(1)

where Z_1 and Z_2 are the atomic numbers of ion and crystal atom, respectively, e is the elementary charge, $a_s = [9\pi^2/(128 Z_2)]^{\frac{1}{3}} a_0$ is the screening radius, and a_0 is the Bohr radius; $\{\alpha_i\} = \{0.10; 0.55; 0.35\}$ and $\{\beta_i\} = \{6.0; 1.2; 0.3\}$ are the fitting parameters and K_0 is modified Bessel function of the zero order and second kind and ρ is the distance between the ion and the Si atom in the transverse plane. The ion-crystal continuum interaction potential is given by the expression, $U_{tot}(\rho) = \sum_{i=1}^{M} U_i(\rho)$, where M is the number of atomics rows taken into account. We take M = 36, i.e. two nearest (relative to the channel axis) triangular coordinate lines.

For the model potential the Hénon-Heiles type potential is used (Hénon & Heiles 1964):

$$V = Z_1 Z_2 e^2 (a(x^2 + y^2) + b(x^3 - 3xy^2))$$
(2)

where a and b are the fitting parameters. The values of the parameters are $a = 4.46 \times 10^{-3}$ and $b = 0.691 \times 10^{-3}$. They are obtained using two independent conditions: (i) frequencies of the transverse motion in the cases of the "exact" and model potentials are equal and (ii) values of the "exact" and model potentials corresponding to the maximum closed equipotential line around the channel axis are equal.

The results presented in this work are obtained using the model potential (2). It is simple, accurate, and efficient considering the computational time.

The transverse components of the ion position, x and y, and ion scattering angle at the exit from the crystal, Θ_x and Θ_y , are determined via the numerical solution of the ion's equations of motion in the transverse plane. The angular distribution of hyperchanneled ions is generated using the computer simulation. The impact parameters of ions are chosen from 2D uniform distribution within the hyperchanneling region. The initial number of ions is around 60 000.

We do not take into account the ion energy loss, the uncertainty of its scattering angle and the change of charge of the ion caused by the collisions with the crystal's electrons since the electron density is low in the hyperchanneling region and the effect of thermal vibrations of the crystal's atoms since the trajectory of the channeled ion is always far away from the atomic strings defining the channel.

3. RESULTS AND DISCUSSION

As it is already mentioned, we study here the dependence of the angular distribution of 60 MeV Ne¹⁰⁺ ion hyperchanneled through the <111> Si crystals on the reduced thickness, that varies from 10 to 21, corresponding to the crystal length from 6.2 to 13.1 μ m.



Figure 1: The angular distributions of 60 MeV Ne^{10+} ions hyperchanneled through the <111> Si thick crystals for the reduced thickness of (a) 10.25, (b) 10.50, (c) 20.25 and (d) 20.50.

Figs. 1 (a)-(d) show the angular distributions of the hyperchanneled ions for variable Λ equal to 10.25, 10.5, 20.25 and 20.5, respectively. Comparing the Figs. 1 (a) with (c) and (b) with (d), it is clear that they are qualitatively similar, thus, showing the periodicity of the angular distribution with the period of 0.5. The values of Λ

= 10, 10.5, 11, ..., 21, correspond to the beginnings of periodic cycles of the angular distribution (Krause et al. 1994; Miletić et al. 1996). The analysis shows that for these values of variable Λ there are pronounced and narrow maxima in the central region of the scattering angle plane i.e. the zero-degree focusing effect occurs (Krause et al. 1994; Miletić et al. 1996).

The angular distribution for $\Lambda = 10.25$ is characterized by the pronounced curved triangular structure in the central region of the scattering angle plane and the pronounced maximum at the origin. For $\Lambda = 10.50$, one can observe that the angular distribution contains the less pronounced curved triangular structure and narrow maximum at the origin and the six "arms" structures lying along the lines $\pi/6 + 2n\pi/6$, where n = 0 - 5. The angular distribution for $\Lambda = 20.25$ is characterized by the pronounced curved triangular structure around the origin and the pronounced maximum at the origin. Also, less pronounced "arms" structures lying along the lines $\pi/6 + 2n\pi/6$, where n = 0 - 5. Finally, for $\Lambda = 20.5$ the angular distribution is characterized by the pronounced narrow maximum at the origin and the six "arms" structures lying along the lines $\pi/6 + 2n\pi/6$, where n = 0 - 5.

It should be noted that the angular distributions presented here have the C_{3V} symmetry which is the consequence of the C_{3V} symmetry of the hyperchanneling region.

One can also observe that the angular distributions for $\Lambda = 10.25$ and 10.5 are characterized by four, and, for $\Lambda = 20.25$ and 20.5, by six symmetrical ridges around the centre of the scattering angle plane. The average distance between the four ridges is larger than the average distance between the six ridges. The analysis of the angular distributions for the values of variable Λ under the consideration confirms observed tendency that the number of ridges increases and the average distance between them decreases as the variable Λ increases. It is interesting to note that the same tendency is recently observed for the angular distributions of 1 GeV protons channelled through the long (11, 9) single-wall carbon nanotubes (Petrović et al.).

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