Nuclear Instruments and Methods in Physics Research B 360 (2015) 23–29

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

# Proton–silicon interaction potential extracted from high-resolution measurements of crystal rainbows

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ARTICLE INFO

*Article history:*
Received 20 May 2015
Received in revised form 21 July 2015
Accepted 21 July 2015

*Keywords:*
Ion channeling
Rainbows
Interaction potential

ABSTRACT

This study provides a way to produce very accurate ion–atom interaction potentials. We present the high-resolution measurements of angular distributions of protons of energies between 2.0 and 0.7 MeV channeled in a 55 nm thick (0 0 1) silicon membrane. Analysis is performed using the theory of crystal rainbows in which the Molière's interaction potential is modified to make it accurate both close to the channel axis and close to the atomic strings defining the channel. This modification is based on adjusting the shapes of the rainbow lines appearing in the transmission angle plane, with the resulting theoretical angular distributions of transmitted protons being in excellent agreement with the corresponding experimental distributions.



## 1. Introduction

Axial ion channeling is the passage of energetic ions through axial crystal channels [1–4], with their trajectories determined by the interaction with crystal atoms. The most frequently used ion–atom interaction potential in treating atomic collisions in solids is that proposed by Ziegler, Biersack & Littmark (ZBL) [5–7]. The other frequently used interaction potential in the field is that derived by Molière [8]. However, the problem of accurate determination of such a potential at small and large ion–atom distances remains acute. Its proper solution will definitively represent an important step forward in many fields, *e.g.*, it will ensure more accurate prediction of impurity concentration profiles during ion implantation processes [9–11], and enable more accurate determination of such profiles [10–12].

Using ion–molecule scattering theory, Nešković [13] and Nešković & Perović [14] developed a model of axial ion channeling in thin crystals, showing that a rainbow occurred. Analogous to scattering of sunlight from water droplets [15,16], the rainbow clearly divided the angular distribution of transmitted ions into the bright and dark parts. In Ref. [17], the model was generalized to be valid for thicker crystals as well. Thus, the theory of crystal rainbows was formulated, allowing accurate investigation of ion channeling in crystals and nanotubes [18].

## 2. Measurements of crystal rainbows

The crystal rainbow effect was first observed experimentally by Krause et al. [19], using protons of an energy of 7 MeV transmitted through (0 0 1) and (0 1 1) silicon crystals that were 140 and 198 nm thick, respectively. The corresponding values of the reduced crystal thickness, defined as $\Lambda = f_k L/v_0$, where $L$ is the crystal thickness, $v_0$ the initial ion velocity, and $f_k$ the frequency of ion motion close to the channel axis, were 0.23 and 0.24, respectively. Since both values of $\Lambda$ were below 0.25, when a majority of ions make less than a quarter of an oscillation around the channel center, the results were analyzed and interpreted using the model of crystal rainbows [13,14]. The authors used the Lindhard's interaction potential [2].

The same group performed another measurement of crystal rainbows [20], using 2–9 MeV protons and 6–30 MeV $C^{4+}$, $C^{5+}$ and $C^{6+}$ ions transmitted through 179 and 190 nm thick (0 0 1) silicon crystals. For protons, the corresponding values of $\Lambda$ were from 0.29 to 0.66, and for carbon ions, they were from 0.29 to 0.85. The results were successfully explained using the LAROSE three-dimensional simulation code [3,21] with the Molière's interaction potential [8]. The authors also analyzed the periodicity of evolution of the whole angular distribution of channeled ions and found that it could be investigated with respect to $\Lambda$, in spite of the fact that the parameter was determined from the second-order terms of the Taylor expansion of the ion–crystal continuum interaction potential close to the axis. They concluded that

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http://dx.doi.org/10.1016/j.nimb.2015.07.104
0168-583X/

the evolution of the angular distribution was to be divided into cycles. The first cycle lasts for $\Lambda$ between 0 and 0.5, the second cycle for $\Lambda$ between 0.5 and 1, and so on.

However, in both experiments, the measurement resolution was not sufficiently high to observe fine structure of the angular distributions of transmitted ions due to inability to provide thinner silicon crystals. Recently, a new silicon crystal fabrication process enabled the production of ultra-thin (001) silicon membranes of a thickness of 55 nm with a surface roughness of 0.4 nm [22]. Those membranes were used in the high-resolution channeling measurements with a 2.0 MeV proton microbeam to study the crystal rainbow effect as well as the doughnut effect [22–25] for the major crystallographic directions. The corresponding value of $\Lambda$ along the [001] direction was 0.12. The same procedure was used to measure the channeling patterns for the minor crystallographic directions [26]. The results were analyzed using the FLUX three-dimensional simulation code [27,28] with the ZBL interaction potential [5–7]. The code uses the binary collision approximation and accounts for the thermal vibrations of crystal atoms and the collisions of protons with crystal electrons.

## 3. Theory of crystal rainbows

Let us now briefly describe the relevant part of the theory of crystal rainbows [17]. We consider that the $z$ axis of the reference frame, being the longitudinal axis, coincides with the channel axis and that its origin lies in the entrance plane of the crystal. The $x$ and $y$ axes of the reference frame, being the transverse axes, are the vertical and horizontal axes, respectively. The initial proton velocity vectors are taken to be parallel to the channel axis. We introduce the mapping of the impact parameter (IP) plane to the transmission angle (TA) plane,

$$\theta_x = \theta_x(x_0, y_0, \Lambda) \text{ and } \theta_y = \theta_y(x_0, y_0, \Lambda), \tag{1}$$

where $x_0$ and $y_0$ are the transverse components of the initial ion position vector, *i.e.*, the components of its impact parameter vector, and $\theta_x$ and $\theta_y$ are the components of the final ion channeling angle, *i.e.*, the components of its transmission angle. To obtain $\theta_x$ and $\theta_y$, the ion equations of motion are solved. It is assumed that the ion–crystal interaction can be treated classically [1–4]. One applies either the continuum approximation [2] or the binary collision approximation [3]. The thermal vibrations of crystal atoms can be included in the calculations.

Since the components of the ion channeling angle remain small during the whole channeling process [1–4], the ion differential transmission cross section is

$$\sigma(x_0, y_0, \Lambda) = \frac{1}{|J_\theta(x_0, y_0, \Lambda)|}, \tag{2}$$

where

$$J_\theta(x_0, y_0, \Lambda) = \partial_{x_0}\theta_x\partial_{y_0}\theta_y - \partial_{y_0}\theta_x\partial_{x_0}\theta_y \tag{3}$$

is the Jacobian of functions $\theta_x(x_0, y_0, \Lambda)$ and $\theta_y(x_0, y_0, \Lambda)$. Hence, equation

$$J_\theta(x_0, y_0, \Lambda) = 0 \tag{4}$$

gives the rainbow lines in the IP plane. The images of these lines determined by functions $\theta_x(x_0, y_0, \Lambda)$ and $\theta_y(x_0, y_0, \Lambda)$ are the rainbow lines in the TA plane.

The theory of crystal rainbows was employed to perform a detailed morphological study of the high-resolution channeling measurements using 2.0 MeV protons and a 55 nm thick (001) silicon membrane tilted away from the [001] direction [25]. It was proved that the doughnut effect was to be considered as the rainbow effect occurring with tilted crystals.

## 4. Interaction potentials

In the field of atomic collisions in solids, the ion–atom interaction potential is of the screened Coulomb type [9]. It can be expressed as $V(R) = V_0(R)\chi(R)$, where $V_0(R) = Z_1Z_2e^2/R$, $Z_1$ and $Z_2$ are the atomic numbers of the ion and crystal atom, respectively, $e$ is the elementary charge, $R$ is the ion–atom distance, and $\chi(R)$ is the ion–atom screening function, describing the effect of electron screening of the atomic nuclei. The screening function is determined using the Thomas–Fermi model or a Hartree–Fock method. In this study, we used the Molière's interaction potential [8], which had been derived from the Thomas–Fermi model, and the ZBL potential, which had been obtained applying an appropriate Hartree–Fock method to 261 atomic pairs [5–7]. The ZBL potential is often designated as the universal potential.

The screening function of the ZBL potential reads

$$\chi_{ZBL}(R) = \sum_{i=1}^{4}\alpha_i \exp\left(-\frac{\beta_i R}{a_{ZBL}}\right), \tag{5}$$

where

$$a_{ZBL} = \frac{(9\pi^2/128)^{1/3}}{Z_1^p + Z_2^p}a_0 \tag{6}$$

is the ZBL screening radius, $a_0$ is the Bohr radius, and $(\alpha_i) = (0.1818, 0.5099, 0.2802, 0.02817)$, $(\beta_i) = (3.2, 0.9423, 0.4028, 0.2016)$ and $p = 0.23$ are the fitting parameters [5–7].

The commonly used form of the screening function of the Molière's potential is

$$\chi_M(R) = \sum_{i=1}^{3}\gamma_i \exp\left(-\frac{\delta_i R}{a_F}\right), \tag{7}$$

where

$$a_F = \frac{(9\pi^2/128)^{1/3}}{\left(Z_1^{1/2} + Z_2^{1/2}\right)^{2/3}}a_0 \tag{8}$$

is the Firsov screening radius, and $(\gamma_i) = (0.10, 0.55, 0.35)$ and $(\delta_i) = (6, 1.2, 0.3)$ are the fitting parameters [8,29]. We denote it as the M($a_F$) potential.

The parameters of the ZBL potential as well as of the M($a_F$) potential were determined to make them accurate dominantly for small ion–atom distances. In analyzing their experimental results, Krause et al. [20] concluded that they were better reproduced by the Molière's potential with the Thomas–Fermi screening radius, being $a_{TF} = (9\pi^2/128)^{1/3}/Z_2^{1/3}a_0$, than by the M($a_F$) potential. We denote it as the M($a_{TF}$) potential. This conclusion was attributed to the fact that each recorded angular distribution of transmitted ions was generated by the ions moving close to the channel axis, *i.e.*, far from the atomic strings defining the channel. One cannot expect a potential that has proven accurate close to the atoms of the strings, *i.e.*, for small ion–atom distances, like the ZBL or M($a_F$) potential, to be accurate close to the channel axis, *i.e.*, for large ion–atom distances, where many atoms influence the ion propagation. The M($a_{TF}$) potential can be written in a form depending on parameter $a_F$, rather than on $a_{TF}$, with parameters $(\delta_i)$ changed to $(\delta_i^c) = (\delta_i a_F/a_{TF})$. For $Z_1 = 1$ and $Z_2 = 14$, $(\delta_i^c) = (5.124, 1.025, 0.2562)$. We denote this potential as the M$^c$($a_F$) potential.

The subject of this study is a sequence of high-resolution measurements performed with 2.0, 1.5, 1.0 and 0.7 MeV focused proton microbeams channeled in a 55 nm thick (001) silicon membrane. Fig. 1 shows the measured angular distributions of transmitted protons of energies of 2.0 and 0.7 MeV together with the corresponding distributions generated using a simulation code based