THE RIANBOW ION-SOLID INTERACTION POTENTIAL

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Abstract

In the article it is reported on the rainbow morphological method to construct an accurate interaction potential, in the case of transmission of 6 MeV protons through <110> Si crystal. The thickness of the crystal was 50 nm. The obtained proton-silicon interaction was named the rainbow interaction potential. It represents extension of the work on the rainbow interaction potential for 27 <100> and <111> cubic crystals: vanadium, chromium, iron, niobium, molybdenum, barium, europium, tantalum, tungsten (BCC crystallographic structure), aluminium, calcium, nickel, copper, strontium, rhodium, palladium, silver, cerium, ytterbium, iridium, platinum, gold, lead and thorium (FCC crystallographic structure), silicon, germanium and tin (diamond type crystallographic structure). Construction of the rainbow interaction potential was based on the fact that it was possible to merge the ZBL interaction potential, for small impact parameters, and the Moliere interaction potential, for large impact parameters, by changing only one fitting parameter in the Moliere interaction potential. Results of the work show that in the case under consideration the same procedure is possible. Moreover, the value of the fitting parameter is close to the values of the same parameter for the <100> and <111> cubic crystals.

1. INTRODUCTION

Recent rapid development of the nanoscience and the nanotechnology imposes new challenges with respect to the basic assumptions considering ion-solid collisions: the energy loss averaging over the impact parameters, the equilibrium charge state distribution and the use of a universal ion-atom interaction potential. The problem of the ion-atom interaction potential will be considered here [1].

The most frequently used ion-atom interaction potential in solids is the ZBL interaction potential [2]. It is based on the so-called universal screening function $a_{ZBL} = (\frac{9\pi^3}{128})^{1/3}(Z_1^p + Z_2^p)^{-1}a_0$, a_0 is the Bohr radius:

$$V_{ZBL} = \frac{Z_1 Z_2 e^2}{R}\sum_{i=1}^{4}\alpha_i \exp\left(-\frac{\beta_i R}{a_{ZBL}}\right), \quad (1)$$

where Z_1 and Z_2 are the atomic numbers of ion and atom, respectively, e is the elementary charge, R is the distance between ion and atom, α_i = (0.1818, 0.5099, 0.2802, 0.02817), β_i= (3.2, 0.9423, 0.4028, 0.2016) and p = 0.23 are the fitting parameters.

Assuming Thomas-Fermi model of atom and its analytical approximation proposed by Moliere [3] one can construct the interatomic potential with the Thomas-Fermi screening radius $a_{TF} = (\frac{9\pi^3}{128})^{1/3}Z_2^{-1/3}a_0$:

$$V_M = \frac{Z_1 Z_2 e^2}{R}\sum_{i=1}^{3}\gamma_i \exp\left(-\frac{\delta_i R}{a_{TF}}\right), \quad (2)$$

where γ_i = (0.10, 0.55, 0.35) and δ_i = (6, 1.2, 0.3) are the fitting parameters. Since the Thomas-Fermi screening radius does not depend on the projectile, which in most cases is not physically feasible, one can introduce the Firsov screening radius $a_F = (\frac{9\pi^3}{128})^{1/3}(Z_1^{1/2} + Z_2^{1/2})^{-2/3}a_0$ [4] getting the same expression (2) by changing δ_i to $\delta_i' = \frac{a_F}{a_{TF}}\,\delta_i$. In this way, it is possible to use expression $V_M = \frac{Z_1 Z_2 e^2}{R}\sum_{i=1}^{3}\gamma_i \exp\left(-\frac{\delta_i' R}{a_F}\right)$, instead of (2). As a result one can include explicitly the influence of the projectile in the screening function.

2. THEORY

In the transmission channeling process one can always define the mapping from the impact parameter plane, which coincides with the entrance plane of a crystal, to the transmission angle plane: $\theta_x = \theta_x(x_0, y_0)$ and $\theta_y = \theta_y(x_0, y_0)$, where x_0 and y_0 are coordinates of the impact parameter of an ion, and θ_x and θ_y are coordinates of its transmission angle. Theory of the crystal rainbow has been developed taking into account that the ion differential transmission cross section for small exit angles of transmitted ions reads [5]:

$$\sigma_{diff}(b) = \frac{1}{|J_\theta(b)|}, \tag{2}$$

where $J_\theta(b) = \partial_{x_0}\theta_x\partial_{y_0}\theta_y - \partial_{y_0}\theta_x\partial_{x_0}\theta_y$ is the Jacobian of the mapping (1). Therefore, the equation: $J_\theta(x_0, y_0) = 0$, defines the rainbow lines in the impact parameter plane. By mappings the rainbow lines in the impact parameter plane one obtains the rainbow lines in the transmission angle plane. It can be shown that all pronounced maxima in the corresponding angular distribution of transmitted ions are determined by the rainbow lines in the transmission angle plane [5-7].

Recently, it has been shown that the rainbow lines can be used to obtain the rainbow interaction potential, which can accurately explain the experimental angular distributions for 0.7-2 MeV protons transmitted through 55 nm thick <100> Si crystal [7]. The used method for the construction of the rainbow potential is based on the following assumptions (i) the ZBL potential is accurate for small impact parameters, (ii) the Moliere potential is accurate for large impact parameters [8], and (iii) the rainbow lines in the scattering angle plane generated by the rainbow potential should match, at the same time, the rainbow lines generated by the ZBL potential, corresponding to small impact parameters, and the rainbow lines generated by the Moliere potential, for the large impact parameters. This method can be named the rainbow morphological method. The remarkable result is that it is possible to obtain the rainbow interaction potential by changing only one parameter in the Moliere potential, δ_2' [7]. This work has been theoretically extended to the case of 27 <100> and <111> cubic crystals: vanadium, chromium, iron, niobium, molybdenum, barium, europium, tantalum, tungsten (BCC crystallographic structure), aluminium, calcium, nickel, copper, strontium, rhodium, palladium, silver, cerium, ytterbium, iridium, platinum, gold, lead and thorium (FCC crystallographic structure), silicon, germanium and tin (diamond type crystallographic structure) [9, 10]. The analysis has shown that for all the <100> cubic crystals, the new parameter δ_2', which is designated by δ_{2r}', is equal to 1.828, while for the <111> cubic crystals, δ_{2r}' = 1.475.

In the work presented here, the method for obtaining the rainbow interaction potential is applied in the case of 6 MeV protons transmitted through 50 nm thick <110> Si crystal.

3. RESULTS

Fig. 1 shows the rainbow lines in the impact parameter plane for <110> Si crystal channel generated in the fitting procedure by the ZBL interaction potential – black line, the Moliere interaction potential – blue line, and the rainbow interaction potential – red line. The channel is a rhomb with symmetric pars of atomic string located around apexes of the rhomb.

Fig. 2 presents the rainbow lines in the angular transmission plane corresponding to the rainbows presented in Fig. 1. It is clear that in the central part of angular transmission plane (larger impact parameters) the rainbow line generated by the rainbow potential is very close to the rainbow line generated by the Moliere potential. In the fitting procedure the corresponding points along the line θ_y = 0 coincide. At the same time, the rainbow line generated by the rainbow potential is very close to the rainbow line generated by the ZBL potential for outer rainbow lines, corresponding to larger angles (smaller impact parameters). Also, in the fitting procedure, the corresponding points along the line θ_y = 0 coincide. Main result is that the fitting procedure requires changing only one parameter in the Moliere interaction potential, as in the cases of <100> and <111> cubic crystals mentioned above, so as δ_{2r}' = 1.388.

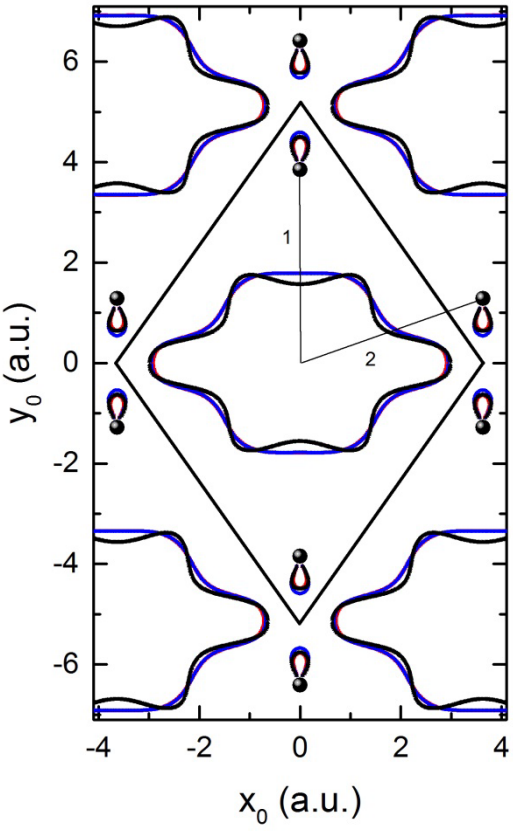

FIG. 1. The rainbow lines in the impact parameter plane generated by the ZBL – black lines, the Moliere – blue lines, and the rainbow interaction potential – red lines. Spheres represent the atomic strings.

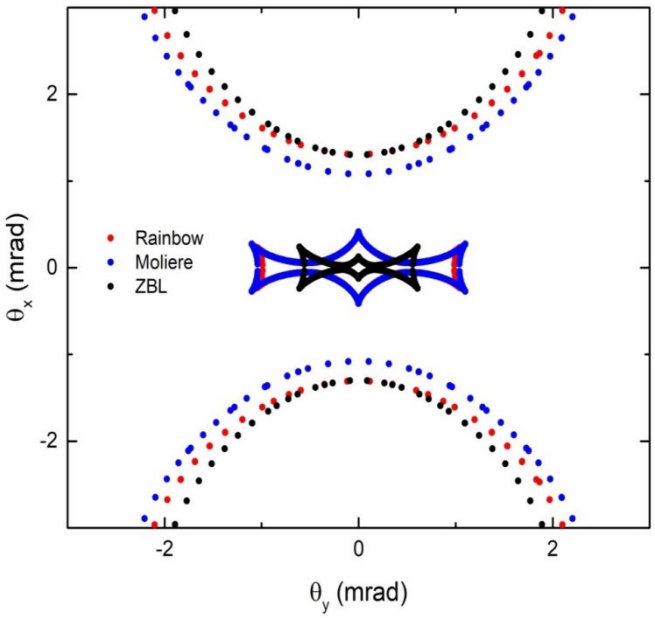

FIG. 2. The rainbow lines in the scattering angle plane generated by the ZBL – black lines, the Moliere – blue lines, and the rainbow interaction potential – red lines.

The comparison between the obtained ZBL, Moliere and rainbow interaction potentials along directions 1 and 2, presented in Fig.1., are shown in Figs. 3 and 4, respectively. In both figures it is clear than the rainbow interaction potential very well approximates the ZBL potential for the small impact parameters while, at the same time, very well approximates the Moliere potential for the large impact parameters. In this way merging of the ZBL and Moliere interaction potentials applying the rainbow morphological method has been achieved.

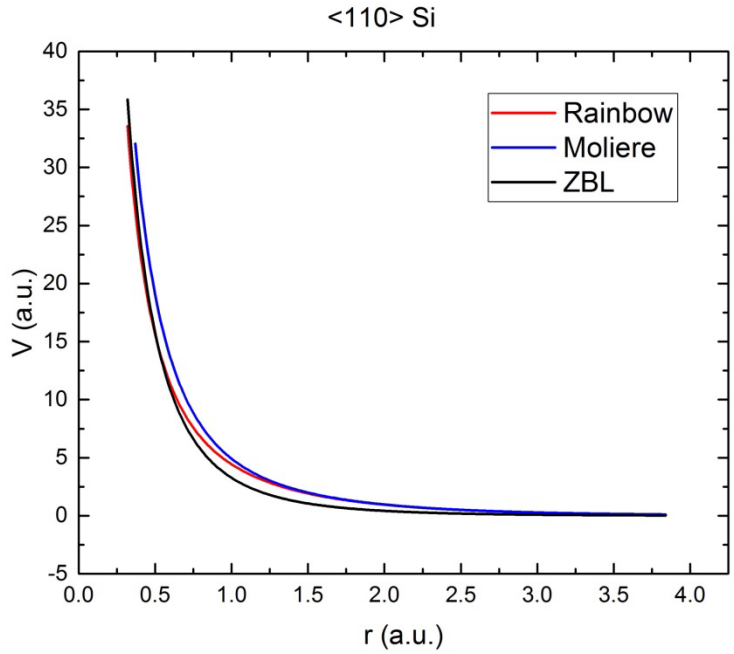

FIG. 3. The rainbow interaction potential – red line, the Moliere interaction potential – blue line, and the ZBL interaction potential – black line, along the direction 1 in Fig.1.

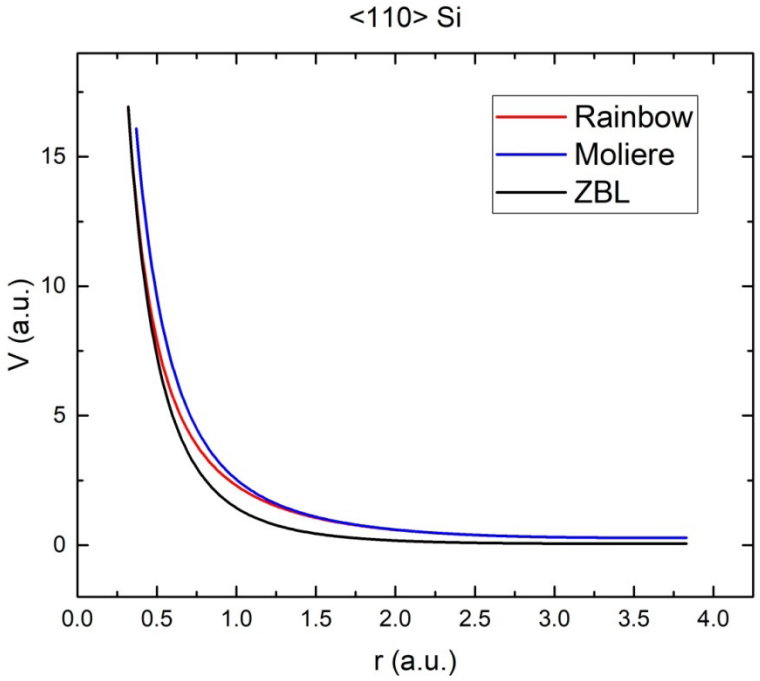

FIG. 4. The rainbow interaction potential – red line, the Moliere interaction potential – blue line, and the ZBL interaction potential – black line, along the direction 2 in Fig.1

4. CONCLUSIONS

The rainbow interaction potential $V_R = \frac{Z_1 Z_2 e^2}{R} \sum_{i=1}^{3} \gamma_i \exp\left(-\frac{\delta'_{ir} R}{a_F}\right)$, with the parameters $\delta'_{ir} = \left(\frac{a_F}{a_{TF}}\ \delta_1, 1.388, \frac{a_F}{a_{TF}}\ \delta_3\right)$, $\delta_1 = 6.0$ and $\delta_3 = 0.3$, has been obtained for the <110> Si crystal applying the rainbow morphological method. It merges the ZBL and the Moliere potential for the whole range of the impact parameters. It should be noted that value of the parameter δ'_{2r} is close to the values of the parameters δ'_{2r} for the <100> and <111> cubic crystals.

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REFERENCES

[1] NASTASI, M., MAYER, J. W., HIRVONEN, J. K., Ion-Solid Interaction: Fundamentals and applications, Cambridge University Press, Cambridge (1996).

[2] ZIRGLER, J. F., BIERSACK J. P., LITTMARK U., The Stopping and Range of Ions in Solids, Pergamon Press, New York (1985).

[3] MOLIERE, G., Theorie der Streuung schneller geladener Teilchen I: Einzelstreuung am abgeschirmten Coulomb-Feld, Z. Naturforsch. A **2** (1947) 133 (in German).

[4] FIRSOV, O. B., Calculation of the interaction potential of atoms, JETP **6** (1958) 534.

[5] PETROVIĆ, S., MILETIĆ, L., NEŠKOVIĆ, N., Theory of rainbows in thin crystals: the explanation of ion channeling applied to Ne10+ ions transmitted through a <100> Si thin crystal, Phys. Rev. B **61** (2000) 184.

[6] MOTAPOTHULA, M., PETROVIĆ, S., NEŠKOVIĆ, N., DANG, Z. Y., BREESE M. B. H., RANA M. A., OSMAN A., Origin of ringlike angular distributions observed in rainbow channeling in ultrathin crystals, Phys. Rev. B **86** (2012) 205426.

[7] PETROVIĆ, S., NEŠKOVIĆ, ĆOSIĆ M., MOTAPOTHULA, M., BREESE M. B. H., Proton-silicon interaction potential extracted from high-resolution measurements of crystal rainbows, Nucl. Instr. Meth. Phys. Res. B **360** (2015) 23.

[8] KRAUSE, H. F., BARRETT, J. H., DATZ, S., DITTNER, P. F., JONES, N. L., GOMEZ del CAMPO, J., VANE, C. R., *Angular distribution of ions axially channeled in a very thin crystal: Experimental and theoretical results*, Phys. Rev. A **49** (1994) 283.

[9] PETROVIĆ, S., STARČEVIĆ, N., ĆOSIĆ M., Universal axial (001) rainbow channeling interaction potential, Nucl. Instr. Meth. Phys. Res. B **447** (2019) 79.

[10] STARČEVIĆ, N., PETROVIĆ, S., Crystal rainbow channeling potential for 〈1 0 0〉 and 〈1 1 1〉 cubic crystallographic crystals, Nucl. Instr. Meth. Phys. Res. B **499** (2021) 39.