THE RIANBOW ION-SOLID INTERACTION POTENTIAL

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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 ZBL universal ion-atom interaction potential.

Petrović et al. [1] presented the high-resolution transmission measurements of the angular distributions of medium energy protons (0.7 – 2 MeV) channeled through a 55 nm thick (001) silicon membrane. They showed that the universal ZBL proton-silicon interaction potential cannot accurately describe the experimental results. As a result, they obtained the rainbow interaction potential (RIP), which approximate ZBL potential for the small impact parameters and the Moliere potential for the large ones. The RIP was constructed by introducing the morphological method based on the crystal rainbow effect [1, 2]. Further, the rainbow morphological method was successfully applied for 27 cubic crystallographic crystals in the (001) and (111) orientations with the BCC crystallographic structure: vanadium, chromium, iron, niobium, molybdenum, barium, europium, tantalum and tungsten; with the FCC crystallographic structure: aluminum, calcium, nickel, copper, strontium, rhodium, palladium, silver, cerium, ytterbium, iridium, platinum, gold, lead and thorium; and the diamond type crystallographic structure: silicon, germanium and tin [3, 4]. For the (001) orientations RIP reds: $V_{001} = \frac{Z_1 Z_2 e^2}{R}\sum_{i=1}^{3}\gamma_i \exp\left(-\frac{\delta_i R}{a_F}\right)$, where the fitting parameters, γ_i = (0.10, 0.55, 0.35), δ_i = (${Z_2}^{1/3}(Z_1^{1/2}+Z_2^{1/2})^{-2/3}$6.0, 1.828, ${Z_2}^{1/3}(Z_1^{1/2}+Z_2^{1/2})^{-2/3}$0.3), while for the (111) orientations, $V_{111} = \frac{Z_1 Z_2 e^2}{R}\sum_{i=1}^{3}\gamma_i \exp\left(-\frac{\delta_i R}{a_F}\right)$, where δ_i = (${Z_2}^{1/3}(Z_1^{1/2}+Z_2^{1/2})^{-2/3}$6.0, 1.475, ${Z_2}^{1/3}(Z_1^{1/2}+Z_2^{1/2})^{-2/3}$0.3) and $a_F = \left(\frac{9\pi^3}{128}\right)^{1/3}(Z_1^{1/2}+Z_2^{1/2})^{-2/3}a_0$ is the Firsov's screening radius. One should note that the obtained potentials differ (for a small amount) for the value of the fitting parameter δ_2 only!

In this work we extend the rainbow morphological method to construct RIP for (110) Si oriented crystal and 6 MeV protons. The channel corresponding to (110) orientation in Si crystal is one of the largest in nature, with can be described by a 2D rhombic Brave crystallographic lattice with two atomic strings per the lattice node.

Figure 1a shows the rainbow lines in the impact parameter plane for RIP, ZBL and Moliere potentials designated by red, black and blue color, respectively. One can observe two separate regions, close to the atomic strings and in between them, corresponding to small and large impact parameters, respectively. It should be note that the rainbow lines in the impact parameter plane, according to the theory of crystal rainbows, are not observable [2, 3]. Figure 2b shows the rainbow lines in scattering angle plane, which has be experimentally established to be a skeleton of the corresponding angular distribution of transmitted channeled ions [1]. It is clear that the rainbow lines corresponding to RIP and ZBL potentials are clearly separate and consequently easily to distinguish in the corresponding experiment.

The analysis shows that for the considered case the fitting parameter δ_2 = 1.388 (the value close to the obtained δ_2 for the above-mentioned cases) and the thickness of the crystal is 50 nm. Therefore, one may hypothesize that an accurate interatomic potential should be the RIP with the average value δ_2 =1.564, for all major crystallographic directions!

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[4] N. Starčević, S. Petrović, Crystal rainbow channeling potential for ⟨1 0 0⟩ and ⟨1 1 1⟩ cubic crystallographic crystals, Nucl. Instrum. Meth. Phys. Res. B 499, 39 (2021).

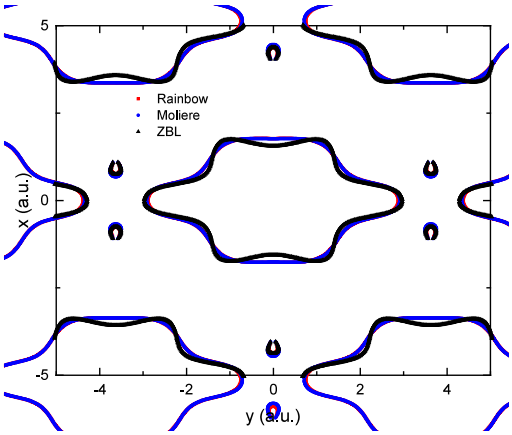

Fig. 1a *Rainbow lines in the impact parameter plane for the, ZBL - black lines, Moliere - blue lines and RIP potentials - red lines for 6 MeV protons and (011) Si crystal.*

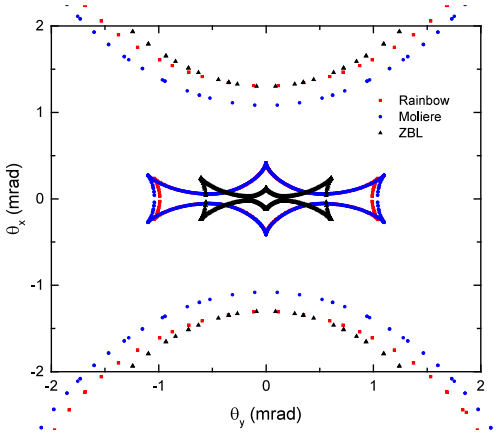

Fig. 1b *Rainbow lines in the scattering angle plane for the, ZBL - black lines, Moliere - blue lines and RIP potentials - red lines for 6 MeV protons and (011) Si crystal.*