

On the shape stability of angular distributions of the channeled protons

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Interaction of Ions with crystals





Figure 1. (a) The simulation of the mean range of 10 keV Si ions in Si. Adapted from *K. Nordlund, F. Djurabekova, G. Hobler, Phys. Rev. B.* **94**, *21*, *214109 (2016)*. (b) Direct intensity distribution on the MCP detector visualizing 50 keV He+ channeling through low-index axes and planes of Si. Adapted from *R. Holeňák, S. Lohmann, D. Primetzhofer, Ultramicroscopy* **217**, *113051 (2020)*.



(a)

(b)

 $\Theta_{\rm c}$

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The channeling effect

The ion-atom interaction potential

$$U_a(r) = \frac{Z_1 Z_2}{r} \sum_i \alpha_i \exp[-\beta_i r / \alpha_{TF}].$$

Continuous potential of atomic string and plane are:

$$U_s(\rho) = \frac{1}{d} \int U_a(r) dz, \qquad U_p(x) = \sigma_p \int U_a(r) dz dy.$$

Ion channel interaction potentials are:

$$U(\boldsymbol{\rho}) = \sum_{n} U_s(\boldsymbol{\rho} - \boldsymbol{\rho}_n), \qquad U(x) = \sum_{n} U_p(x - x_n).$$

One just needs to solve the Hamilton equations of motion:

$$\frac{\mathrm{d}\boldsymbol{\theta}}{\mathrm{d}t} = -\frac{\nabla_{\boldsymbol{\rho}}}{p_z}H(\boldsymbol{\rho},\boldsymbol{\theta}), \qquad \frac{\mathrm{d}\boldsymbol{\rho}}{\mathrm{d}t} = \frac{\nabla_{\boldsymbol{\theta}}}{p_z}H(\boldsymbol{\rho},\boldsymbol{\theta}),$$
$$H(\boldsymbol{\rho},\boldsymbol{\theta}) = \frac{p_z^2}{2m}\boldsymbol{\theta}^2 + U(\boldsymbol{\rho}),$$

The critical channeling angles

$$\Theta_c = \sqrt{\frac{2m}{p_z^2}} U_s(a_{TF}), \qquad \Theta_c = \sqrt{\frac{2m}{p_z^2}} U_p(d_p - a_{TF}),$$

Figure 2 (a) Scattering on an atomic string. (b) Schematic representation of the channeling effect.

 (θ_x, θ_y)

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The Statistical Equilibrium Hypothesis

The channeled trajectories are very complicated; thus, it is *assumed* that ion beam quickly reaches the transverse equilibrium state!

In the planar case integral curves can be labeled by impact parameters x_o .

The corresponding microcanonical distribution is $S(H(x, \theta_{-}) - H(x, \theta_{-}))$

$$w(x, \theta_x; x_0) = \frac{\delta(H(x, \theta_x) - H(x_0, 0))}{\int \delta(H(x, \theta_x) - H(x_0, 0)) \mathrm{d}x \mathrm{d}p_x'}$$

Phase space distribution of the beam is $W(x, \theta_x) = \frac{1}{d_p} \int_{-d_p/2}^{d_p/2} w(x, \theta_x; x_o) dx_0,$

with angular distribution

$$Y(\theta_x) = \int_{-d_p/2}^{d_p/2} W(x, \theta_x) dx_0$$

Figure 3. Ergodic angular density for model of planar interaction potential $U(x) = U_0 \cos qx$. Adapted from the M. V. Berry D. O'Dell, J. Phys. A: Math. Gen. **32** 3571–3582 (1999).





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Angular Distributions in thin Crystal

Unfortunately, the channeled beam is never ergodic!



Figure 4. Experimental channeled angular distributions at aligned cases for 2 MeV protons from a 55 nm [001] Si membrane, doughnut channeling patterns. Adapted from *M. Motapothula, Z. Y. Dang, T. Venkatesan, M. B. H. Breese, Nim Phys. Res. B* **330** 24–32, (2014).

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Crystal Rainbow Effect

The axial channeling process is a map of the impact parameter plane to the scattering angle plane

 $\boldsymbol{\rho}_{\mathbf{0}} = (x_0, y_0) \stackrel{\Lambda}{\to} \boldsymbol{\theta} = (\theta_x, \theta_y),$ parametrized by the reduced crystal thickness $\Lambda = \frac{t}{T} = \frac{L}{2\pi} \sqrt{\Delta U(0)/E_k}$. The differential cross-section is $\sigma_{\rm diff}(\boldsymbol{\theta}, \Lambda) = \frac{1}{|\boldsymbol{J}_{\boldsymbol{\theta}}(\Lambda)|}, \qquad \boldsymbol{J}_{\boldsymbol{\theta}} = \begin{vmatrix} \partial_{\boldsymbol{\chi}_0} \theta_{\boldsymbol{\chi}}(\boldsymbol{\rho}_0, \Lambda), & \partial_{\boldsymbol{\chi}_0} \theta_{\boldsymbol{\chi}}(\boldsymbol{\rho}_0, \Lambda) \\ \partial_{\boldsymbol{\chi}_0} \theta_{\boldsymbol{\chi}}(\boldsymbol{\rho}_0, \Lambda), & \partial_{\boldsymbol{\chi}_0} \theta_{\boldsymbol{\chi}}(\boldsymbol{\rho}_0, \Lambda) \end{vmatrix}.$ 0.7 MeV 1.0 MeV 0.2 (deg) 0 θ_{χ} -0.2 min -0.2 0 0.2 -0.2 0 0.2 θ_{v} (deg)

Figure 5. Experimental angular distribution of 1.0, and 0.7-MeV protons transmitted through 55nm long (100) channel Si crystal with corresponding rainbow lines (red lines).

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Proton's isoenergy contours



Figure 6. (a) Inequivalent isoenergy contours in the impact parameter plane, whose energies are shown in the inset (a'). (b), (c) an image of isoenergy lines in (ρ , θ_x) space for Λ = 0.164 and 0.468. Black diamonds show the positions of the atomic strings, while the black circle indicates the center of the axial channel. Arrows indicate contours belonging to the hyper-channeled manifold.

The Experiment





Figure 7. (a) The schematic representation of the experimental setup installed at the μ -beam line of the Ruđer Bošković Institute.

(b) Antiblocking pattern captured by the forward scattering detector. Arrows indicate the positions of the planar channels, the dashed circle axial channel. The number of detected protons was represented by color ranging from the deepest blue to the deepest red.

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Crystal Rainbow Effect



Figure 8. (a)-(c) Measured angular distribution of transmitted protons for $\Lambda = 0.597$, 0.468, and 0.372. Arrows indicate inequivalent accumulation regions and the extent of the distribution. (a')-(c') The corresponding projections of the isoenergy contours to the scattering angle plane



Conclusions

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- There seem to be certain, practically perpetually stable, isoenergy lines for which perturbations can't overpower the influence of the correlated sequence of the small-angle scattering.
- Regardless of having measure zero, stable isoenergy lines provide organizing centers for the dynamics on all neighboring, unstable isoenergy lines, thus enabling the shape consistency of their projections into the SA plane to become observable.
- The stable iso-energy lines are the last feature of the angular distributions of channeled protons to be erased by the nonelastic effects.

