Ion Channeling and Catastrophe Theory

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The rainbow effect in ion channeling (in very thin crystals) is considered. In the analysis the results of catastrophe theory are used. The calculations were performed for 10-MeV H^+ ions and the ⟨100⟩ channel of a 1000-Å-thick Au crystal.

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It has been shown recently[1] that in ion channeling in very thin crystals the differential transmission cross section is singular, i.e., the rainbow effect occurs. This was explained by the fact that contributions of the atomic strings of the crystal to the differential transmission cross section interfere. Shortly after the prediction the effect was observed.[2] In this Letter we shall consider the rainbow effect in ion channeling in the case of 10-MeV H^+ ions and the ⟨100⟩ channel of a 1000-Å-thick Au crystal. The results obtained will be compared to the corresponding ones given by catastrophe theory.[3] It should be noted that a similar effect, occurring in particle scattering from surfaces, was analyzed by Berry.[4]

The z axis is taken to coincide with the channel axis and the origin to lie in the median plane of the crystal. The incident ion velocity is parallel to the z axis. The crystal is assumed to be sufficiently thin for the ion trajectory to be approximated by a straight line. In this case the components of the scattering angle and the differential transmision cross section as functions of the impact parameter can be easily obtained with use of the momentum approximation.[1] We assume that the ion-atom interaction potential is of the Thomas-Fermi type; for the integral of that potential along the trajectory, needed in applying the momentum approximation, we use Lindhard's expression,[5]

$$V_i = Z_1 Z_2 e^2 \ln\left[\frac{Ca_s^2}{(x-x_i)^2+(y-y_i)^2}+1\right], \qquad (1)$$

where Z_1 and Z_2 are the atomic numbers of the ion and the crystal, respectively. x and y are the components of the impact parameter, x_i and y_i are the transverse coordinates of the atoms of the ith atomic string of the crystal, $a_s = (9\pi^2/128Z_2)^{1/3}a_0$ is the screening radius, a_0 is the Bohr radius, and $C=3$ is a fitting parameter. Variable V_i/Z_1ed, where d is the distance between the atoms of the atomic strings, is the continuum potential of the ith string.[5]

As has been said above, we consider here 10-MeV H^+ ions in the ⟨100⟩ channel of a 1000-Å-thick Au crystal. Since in this case the distance between the atoms of the atomic strings of the crystal equals the unit-cell parameter, which is 4.078 97 Å,[6] the number of atoms in one atomic string is 246. The number of strings is 24, i.e., we take into account the strings lying on the four nearest (relative to the channel center) coordination circles.[1] Figure 1 gives the rainbow line, i.e., the line along which the differential transmission cross section is singular, in the impact-parameter plane in this $H^+ \rightarrow$ Au case. The coordinates of the atomic strings lying on the first coordination circle, in a.u., are (2.73,0), (0,2.73), (−2.73,0), and (0,−2.73). The coordinates of the points defining this line are determined only by the arrangement of the atomic strings and the continuum string potential[1]; they do not depend on the atomic number of the ion, ion energy, and crystal thickness. This figure also gives the rainbow line in the scattering-angle plane. The line has four cusps, each of them directed towards an atomic string lying on the first coordination circle, and lies in the region in which the scattering angle is smaller than 0.73 mrad;

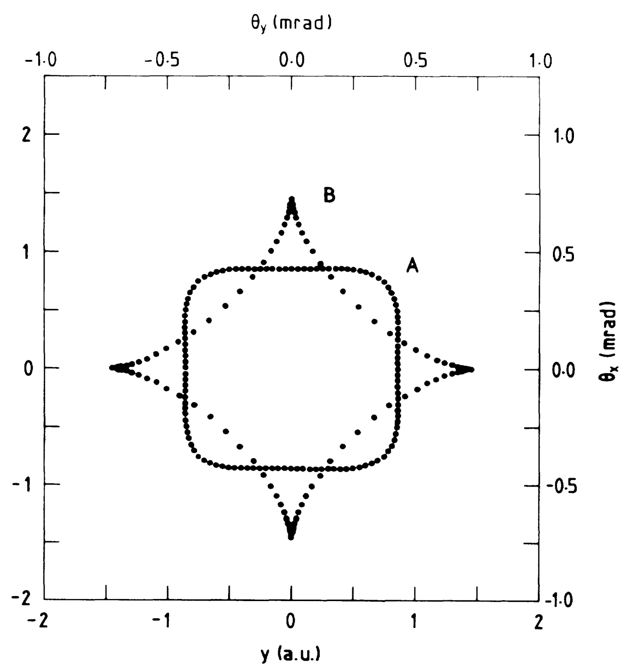

FIG. 1. A, the rainbow line in the impact-parameter plane; B, the rainbow line in the scattering-angle plane.

the corresponding (maximal) distance traveled by the ion in the transverse plane is 0.69 a.u. The fact that the ratio of this distance and the radius of the first coordination circle is 0.25 justifies the use of the momentum approximation.[1,2] The coordinates of the points defining the rainbow line in the scattering-angle plane depend on the atomic number of the ion, ion energy, and crystal thickness.[1] However, the ratios of these coordinates and $Z_1eN/2E$, where E is the ion energy and N the number of atoms in one atomic string, do not depend on these parameters.[1] This means that the shape of this line is determined only by the arrangement of the atomic strings and the continuum string potential, i.e., by the continuum potential in the channel.

It is clear that the components of the scattering angle, θ_x ane θ_y, are single-valued functions of the components of the impact parameter (x and y). On the other hand, variables x and y are complicated multiple-valued functions of θ_x and θ_y. These functions can be obtained by the computer simulation method. Values of variables x and y are chosen randomly or uniformly within the region of the channel and, according to the calculated values of θ_x and θ_y and chosen values of x and y, each ion is recorded as if it entered a bin in the $\theta_x\theta_y x$ space and a bin in the $\theta_x\theta_y y$ space. Thus, for a large number of ions, we obtain for one bin in the scattering-angle plane (the $\theta_x\theta_y$ space) the distributions of variables x and y. The number of maxima of these distributions represents the number of values of functions x and y for this particular bin. The angular distribution of the transmitted ions[1,2] is obtained by summation of the contents of the bins in the $\theta_x\theta_y x$ space or in the $\theta_x\theta_y y$ space corresponding to each bin in the scattering-angle plane. Here, we present the analysis of function $y(\theta_x,\theta_y)$ in the vicinity of the apex of the cusp of the rainbow line lying in the fourth and first quadrants of the scattering-angle plane. The change of function $x(\theta_x,\theta_y)$ in this region, along the rainbow line, is very small (see Fig. 1) and, therefore, less interesting; we shall consider it elsewhere.[7] The sizes of a bin in the $\theta_x\theta_y y$ space along the θ_x and θ_y axes were equal to 0.02 mrad, and its size along the y axis was equal to 0.04 a.u. Values of variables x and y were chosen uniformly, and the number of ions was $\simeq 9\times 10^5$. Figure 2 gives the changes of function y with variable θ_y for three values of θ_x: 0.51, 0.65, and 0.79 mrad. The comparison of this figure to Fig. 1 shows that function $y(\theta_x,\theta_y)$ is triple valued on the inner side of the rainbow line and single valued on its outer side. Besides, it is clear that y is an odd function of θ_y.

The aim of this study is to compare the shapes of the rainbow line in the scattering-angle plane and the surface defined by function $y(\theta_x,\theta_y)$ in the vicinity of the apex of the cusp of the rainbow line lying in the fourth and first quadrants of the scattering-angle plane to the corresponding shapes given by catastrophe theory.[3,8,9] The assumption is that the singularity of the differential transmission cross section we have is an elementary catastrophe, and that in the case under consideration (the

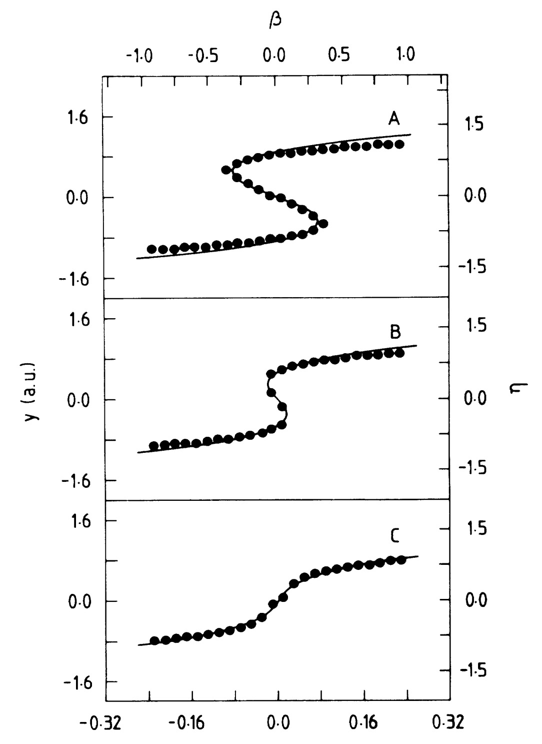

FIG. 2. The changes of function y with variable θ_y for three values of θ_x obtained by the computer simulation method (solid circles), and by Eq. (3) (solid lines); (a) θ_x =0.51 mrad, (b) θ_x =0.65 mrad, (c) θ_x =0.79 mrad.

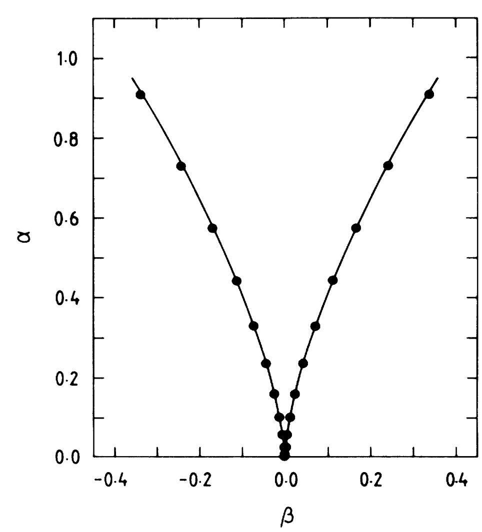

FIG. 3. The rainbow line in the scattering-angle plane in the vicinity of the apex of the cusp (solid circles), and the line defined by Eq. (2) (solid line).

case of ⟨100⟩ channel of an Au crystal) it is the cusp catastrophe. For the control variables we take $\alpha=-(\theta_x-\theta_{xc})/\theta_0$ and $\beta=\theta_y/\theta_0$, where θ_{xc} is the value of variable θ_x corresponding to the apex of the cusp and $\theta_0=k_\theta Z_1 Z_2 e^2 N/2Ed$; for the behavior variable we take $\eta=y/\rho_0$, where $\rho_0=k_\rho d$; k_θ and k_ρ are the scaling factors. According to catastrophe theory the line corresponding to the rainbow line in the vicinity of the apex of the cusp is determined by[3,8]

$$\alpha=3\,|\beta/2\,|^{2/3}. \quad (2)$$

The surface corresponding to the one defined by the function $y(\theta_x,\theta_y)$ is given by the equation

$$\eta^3-\alpha\eta-\beta=0, \quad (3)$$

and the lines separating the "branches" of this surface are given by

$$\eta=\pm(\alpha/3)^{1/2}. \quad (4)$$

Figure 3 gives the comparison of the shapes of the rainbow line in the vicinity of the apex of the cusp and the line defined by Eq. (2). Each branch of the rainbow line is given by twelve points, corresponding to the points in the impact-parameter plane with y coordinates between 0 and ± 0.55 a.u. with the step of 0.05 a.u. (the x coordinates of these points are smaller than zero). The last point of each branch of the rainbow line is chosen so that the ratio of its α coordinate and α_m, the α coordinate of the midpoint of the rainbow line between the cusp under consideration and the neighboring cusp, is smaller than and close to 0.5. The value of the scaling factor k_θ is 0.0717; it is determined by the condition that the average ratio of the α coordinates of the points of the rainbow line and the corresponding points of the line given by Eq. (2) is equal to 1. In order to measure the difference between the shapes of these lines we introduce parameter ϵ_θ, the square root of the average square relative difference between the α coordinates of the points of these lines; in this case it equals 0.537%. The comparison of the shapes of the surfaces defined by functions $\eta(\alpha,\beta)$ obtained by the computer simulation method and by Eq. (3) is shown in Fig. 2; the values of variable α are 0.886 (curve A), 0.317 (curve B), and -0.253 (curve C). The value of the scaling factor k_ρ will be given later on. Figure 4 shows the comparison of the shapes of the lines separating the branches of the surfaces under consideration. Each branch of the line obtained by the computer simulation method is given by eleven points, whose α coordinates are determined by θ_x coordinates between 0.51 and 0.71 mrad with the step of 0.02 mrad. The last point of each branch of this line, as in the case of the rainbow line, is chosen so that the ratio of its α coordinate and α_m is smaller than and close to 0.5. The scaling factor k_ρ and parameter ϵ_ρ, introduced to measure the difference between the shapes of the lines under consideration, are determined in the analogous way as in the case of the rainbow line; their values are 0.120 and 9.45%, respectively.

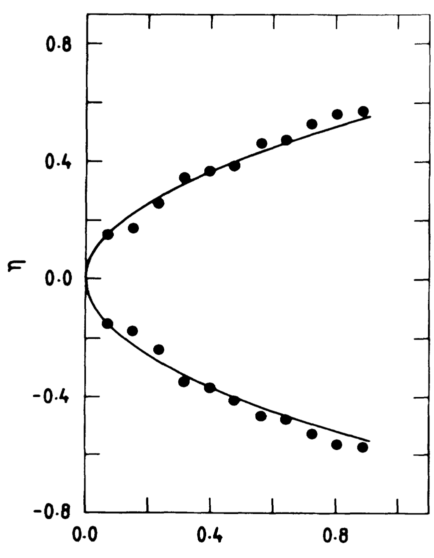

FIG. 4. The lines separating the branches of the surfaces defined by functions $\eta(\alpha,\beta)$ obtained by the computer simulation method (solid circles), and by Eq. (4) (solid line).

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[1]N. Nešković, Oak Ridge National Laboratory Report No. 6004, 1983 (unpublished), p. 203, and Phys. Rev. B **33**, 6030 (1986).

[2]H. F. Krause, S. Datz, P. F. Dittner, J. Gomez del Campo, P. D. Miller, C. D. Moak, N. Nešković and P. L. Pepmiller, Phys. Rev. B **33**, 6036 (1986).

[3]R. Thom, *Structural Stability and Morphogenesis* (Benjamin, Reading, MA, 1975).

[4]M. V. Berry, J. Phys. A **8**, 566 (1975).

[5]J. Lindhard, K. Dan. Vidensk. Selsk., Mat.-Fys. Medd. **34**, No. 14 (1965).

[6]J. D. H. Donnay and H. M. Ondik, *Crystal Data Determinative Tables* (U.S. G.P.O., Washington, D.C., 1973), Vol. 2, p. C-44.

[7]N. Nešković and B. Perović, to be published.

[8]Th. Bröcker, *Differentiable Germs and Catastrophes* (Cambridge Univ. Press, Cambridge, 1975), p. 144.

[9]M. V. Berry, Adv. Phys. **25**, 1 (1976).