SOVIET PHYSICS JETP VOLUME 31, NUMBER 1 JULY, 1970

THEORY OF CHANNELING EFFECT. I

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Submitted June 18, 1969

Zh. Eksp. Teor. Fiz. 58, 226–244 (January, 1970)

A consistent method for analysis of channeling and related effects is developed. It is based on the density-matrix formalism and permits one to single out in a consistent manner coherent diffraction due to regularity of the medium. In the case of plane channeling and neglect of inelastic scattering, the problem reduces to that of motion of a particle in a one-dimensional periodic potential $V_{eff}(x)$ that depends on the crystal temperature. States whose energies are close to the maximal values of $V_{eff}(x)$ are found to play an important role. The distance from the input surface, over which a significant change of the nuclear reaction yield occurs, is studied. It is shown that spikes of the nuclear reaction yield can appear with increase of the crystal thickness (resembling an "echo"). A concrete analysis is carried out for a model potential of the Kronig-Penney type. The calculations yield all the qualitative results, and in particular reveal quantum oscillations of the nuclear-reaction yield, averaged over the thickness, as a function of the angle of incidence.

1. INTRODUCTION

RECENTLY an interesting class of phenomena has been revealed, connected in one manner or another with the appreciable influence of the periodicity in the arrangement of the atoms on the character of motion of fast heavy charged particles in a crystal. It has turned out that such a motion cannot be regarded as multiple uncorrelated scattering by individual centers. To the contrary, under certain conditions, the correlation in the scattering by individual atoms becomes very strong, radically altering the character of the occurring processes. This is most clearly manifest in a phenomenon called the channeling effect. This effect consists in the fact that the intensity of the nuclear reaction[1,2] and of the large-angle scattering[3,4] increases sharply for particles moving in a narrow angle interval along the crystallographic axis ("axial channeling") or the crystallographic planes ("planar channeling"), and a radical change takes place in the character of the energy loss and the angular distribution of the scattered particles compared with an amorphous body (see, for example,[5-7]).

Theoretical considerations explaining how a periodic structure changes the picture of the interaction of the fast charged particles with matter, were advanced by Lindhard[8]. His analysis is based on an examination of the classical scattering of a particle by a one-dimensional chain of atoms, when the trajectory of the particles and the chain lie in the same plane. He called attention to the fact that in scattering by a single atom at a small angle of incidence relative to the chain, the next atom is, as it were, in the "shadow" of the preceding one, and effective "squeezing" (in the case when the particle is positively charged) of the particle trajectory away from the chain takes place, thereby hindering collisions with a small impact parameter. Lindhard replaced the chain of atoms by a continuous uniform filament producing a certain axially-symmetrical potential, and estimated for this model the limiting angle at which the particle can still not penetrate into the space in the direct vicinity of the filament.

The model based on introducing an average potential and considering classical scattering was further developed, in particular, by Erginsoy[9]. Erginsoy went farther, and considered for the first time planar channeling, introducing a potential averaged over the atomic planes and estimating the corresponding limiting angle (the "channeling angle").

These very simple models, which admit in particular of a certain generalization to take the oscillations of the atoms into account, have made it possible to understand qualitatively the main results and to obtain estimates of the experimental parameters.

De Wames et al.[10] attempted to present a quantum-mechanical description of the phenomenon. The analysis was based on the use of the formalism of dynamic diffraction for particles described by the Schrodinger equation (see[11]), and the channeling effect was treated as a certain analog of the Bormann effect, which is known in the theory of x-rays. This paper gave rise to a discussion[12,14], and was subject to a criticism. On one hand, it was correctly noted that the employed approximation of two or three waves is certainly not appropriate for the problem[14] (this will be shown very clearly in what follows), and on the other hand it was indicated that the process of essentially inelastic (incoherent) scattering leads to a contradiction with the usual form of the analysis of stationary dynamic diffraction[12]. Unfortunately, the discussion reduced mainly to an ineffective discussion of the question of the relation between classical and quantum aspects of the phenomenon, and the theory received practically no further development (see also[15,16]).

In this paper we develop a method for analyzing the channeling effect and related phenomena, based on the use of the density-matrix formalism. This method makes it possible to separate consistently the coherent diffraction generated by the regularity of the medium, and, in principle, makes it also possible to take into account the incoherent inelastic scattering with excitation of the degrees of freedom of the crystal.

Within the framework of the considered method, it is possible to explain in the unified fashion all the observed phenomena, and in particular, it is possible to reveal naturally their quantum and classical aspects. We present in this paper the results obtained with inelastic processes neglected.

2. INITIAL RELATIONS

Let a fast charged particle move in a crystal. The Hamiltonian describing this system can be presented in the form

$$\hat{H} = \hat{H}_1 + \hat{H}_2, \tag{2.1}$$

where $\hat{H}_1$ is the Hamiltonian of the particle, taking into account its interaction with the crystal, and $\hat{H}_2$ is the total Hamiltonian of the crystal.

We introduce the total density matrix $\hat{\rho}$ for the entire system as a whole. The equation for it has the usual form ($\hbar = 1$)

$$i\partial\hat{\rho} / \partial t = [\hat{H}, \hat{\rho}]. \tag{2.2}$$

Neglecting the influence of the particle in the state of the crystal, we can represent the density matrix in the form of the product $\hat{\rho}_1\hat{\rho}_2$, where $\hat{\rho}_1$ is the density matrix operating in the function space of the particle, and $\hat{\rho}_2$ is the density matrix of the crystal. The latter as usual, will be assumed to be diagonal in the representation of the eigenfunctions of H_2. Then, taking the trace of both parts of (2.2) with respect to the variables of the crystal, we have

$$i\partial\hat{\rho}_1 / \partial t = [\hat{H}_0, \hat{\rho}_1] + \mathrm{Sp}_2[\hat{H}_1 - \hat{H}_0, \hat{\rho}_1\hat{\rho}_2], \tag{2.3}$$

where

$$\hat{H}_0 = \mathrm{Sp}_2(\hat{\rho}_2\hat{H}_1) \tag{2.4}$$

is the Hamiltonian of a particle moving in the averaged and consequently strictly periodic potential of the crystal.

We write the Hamiltonian $\hat{H}_1$ in the form

$$\hat{H}_1 = \hat{\mathbf{p}}^2/2M + \hat{V}(\mathbf{r}), \quad \hat{V}(\mathbf{r}) = \sum_m \hat{V}_m(\mathbf{r}) \tag{2.5}$$

(the index m numbers the atoms in the crystal), and use for $\hat{V}(\mathbf{r})$ the Fourier representation

$$\hat{V}(\mathbf{r}) = \sum_{\mathbf{q}, m} \hat{V}_{\mathbf{q}, m} e^{i\mathbf{q}(\mathbf{r}-\mathbf{R}_m)}. \tag{2.6}$$

Here $\hat{V}_{q,m}$ is the operator acting on the variables of the individual atom, whose matrix elements coincide with the matrix elements corresponding to the Born scattering of the charged particle with transfer of momentum q to the atom; R_m is the coordinate of the m-th nucleus.

It is seen from (2.6) that the averaging of (2.4) reduces to an averaging of $\hat{V}_{q,m} \exp(-iq \cdot R_m)$. In turn, the averaging of $\hat{V}_{q,m}$ reduces obviously to taking the diagonal matrix element over the ground state of the m-th atom. The corresponding value will be designated simply as

$$V_{\mathbf{q}, m} \equiv (\hat{V}_{\mathbf{q}, m})_{00}. \tag{2.7}$$

We introduce the displacement u_m from the equilibrium position of the atom r_m. We then obtain directly

$$\mathrm{Sp}_2(\hat{\rho}_2\hat{V}_{\mathbf{q}, m} e^{-i\mathbf{q}\mathbf{R}_m}) = V_{\mathbf{q}, m} e^{-i\mathbf{q}\mathbf{r}_m} e^{-Z_m(\mathbf{q})/2} \tag{2.8}$$

where

$$Z_m(\mathbf{q}) = \langle(\mathbf{q}\mathbf{u}_m)^2\rangle \tag{2.9}$$

coincides with the argument of the exponential in the Debye-Waller factor (the index $\langle \ldots \rangle$ corresponds to averaging over the thermal equilibrium).

Substituting the obtained expressions in (2.4) and recognizing that $\Sigma \exp(-iq \cdot r_m)$ in a regular crystal differs from zero only if q coincides with **K** (the reciprocal-lattice vector multiplied by 2π), we obtain ultimately

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2M} + \frac{1}{\Omega_0} \sum_{\mathbf{K}} \sum_{i} V_{\mathbf{K}, j} e^{-Z_j(\mathbf{K})/2} e^{-i\mathbf{K}\mathbf{r}_j} e^{i\mathbf{K}\mathbf{r}}. \tag{2.10}$$

Here Ω_0 is the volume of the unit cell, and the sum over j is the sum over the atoms of the individual unit cell.

Thus, $\hat{H}_0$ describes the motion of a particle in a periodic potential $\overline{V}(\mathbf{r})$, whose Fourier components are equal to

$$\overline{V}_{\mathbf{K}} = \frac{1}{\Omega_0} \sum_j V_{\mathbf{K}, j} e^{-Z_j(\mathbf{K})/2} e^{-i\mathbf{K}\mathbf{r}_j}. \tag{2.11}$$

In analyzing the real problem, it is necessary to consider the boundary-value problem, and as the boundary condition we must assume that the ψ-function of the incident particle on the input surface coincides with a plane wave. However, if account is taken of the classical character of the motion of the fast particle in the crystal along the direction of incidence, then we can consider in lieu of the boundary problem an equivalent temporal problem, assuming that the interaction of the particle with the crystal is turned on at the instant of time $t = 0$, and considering the evolution of the motion of the particles with time in an infinite crystal. It is then obvious that for a thin real crystal we have a one-to-one correspondence between the time t and the thickness coordinate z.

We shall henceforth operate in the representation of the eigenfunctions $\psi_S(\mathbf{r})$ of the Hamiltonian $\hat{H}_0$. If we expand the plane wave in the functions $\psi_S(\mathbf{r})$, then we get for the coefficients $C_S(\mathbf{q})$ in this expansion

$$C_s(\mathbf{q}) = \int e^{i\mathbf{q}\mathbf{r}} \psi_s^*(\mathbf{r})\, d\mathbf{r}. \tag{2.12}$$

If q coincides with the wave vector of the incident particles, then the initial condition for the density matrix is written in the form

$$\rho_{1s_1s_2}(0) = C_{s_1}(\mathbf{q}) C_{s_2}^*(\mathbf{q}). \tag{2.13}$$

The solution of Eq. (2.3) with the initial condition (2.13) makes it possible to find all the quantities of interest to us. Indeed, to determine the yield of a nuclear reaction at a definite depth, or of the scattering of particles through large angles, it is necessary to know the microscopic density of the fast particles near the nuclei of the crystal. As to the density, we have for it in the general case the following expression:

$$n(\mathbf{r}, t) = \sum_{s_1, s_2} \rho_{1s_1s_2}(t) \psi_{s_1}(\mathbf{r}) \psi_{s_2}^*(\mathbf{r}). \tag{2.14}$$

The energy distribution function $g(E, t_0)$ of the particles after passing through a crystal of thickness $z_0(t_0)$ can be represented in the form

$$g(E, t_0) = \sum_s \rho_{1ss}(t_0) \delta(E - E_s). \tag{2.15}$$

Here E_S is the eigenvalue of the Hamiltonian $\hat{H}_0$. (We neglect here the renormalization of the particle energy as a result of the inelastic processes.)

The mean value of the energy losses is

$$\Delta E(t_0)=\sum_s E_s[\rho_{1ss}(0)-\rho_{1ss}(t_0)]. \tag{2.16}$$

To find the angular distribution of the particles it is necessary to determine the distribution on the particles with respect to the final momentum. But the latter quantity is simply the diagonal element ρ_{1KK} of the density matrix, determined in the plane-wave representation. Using (2.12), we readily find

$$\rho_{1\varkappa\varkappa}(t_0)\equiv\rho_1(\varkappa, t_0)=\sum_{s_1,s_2} C^*_{s_1}(\varkappa)\, C_{s_2}(\varkappa)\,\rho_{1s_1s_2}(t_0). \tag{2.17}$$

The angular distribution of the particles is determined in this case by

$$\rho_1(\mathbf{n}_\varkappa, t_0)=\int\rho_1(\varkappa, t_0)\frac{\varkappa^2 d\varkappa}{(2\pi)^3}, \qquad \mathbf{n}_\varkappa=\frac{\boldsymbol{\varkappa}}{\varkappa}, \tag{2.18}$$

and the expression (2.17) itself yields, apart from the factor, the energy distribution of the particles after passing through the crystal in the n_K direction.

3. MOTION OF FAST PARTICLE IN A PERIODIC POTENTIAL

The motion of a particle in the averaged lattice potential is described by a dynamic system of equations obtained directly from the Schrödinger equation (see[11]):

$$(E_\mathbf{q}-E)\,\psi_\mathbf{q}+\sum_\mathbf{K}\overline{V}_\mathbf{K}\psi_{\mathbf{q}-\mathbf{K}}=0, \tag{3.1}$$

$$E_\mathbf{q}=\mathbf{q}^2/2M. \tag{3.1$'$}$$

Here ψ_q is the Fourier component of the ψ-function of the particle, and V_K is defined in accordance with (2.11).

The main question of interest to us is that of the possible appreciable modification of the ψ-function for particles whose energy E is large compared with the periodic potential. In other words, we are dealing with the possibility of the reconstruction of the particle into a quasiparticle whose properties can differ in principle from those of the particle. It must be stated that for heavy particles that interact weakly with the atoms of the crystal, when the wavelength λ is comparable with the interatomic distance a, there is indeed a strong modification of the ψ-function under definite conditions[11]. Thus, for a neutron with wave vector q lying near the boundary of the Brilouin zone, the state in the crystal represents a super-position of two plane waves differing by the reciprocal-lattice vector. The neutron in such a state interacts with the nuclei in an entirely different manner than the free particle, as a result of which, in particular, the inelastic channels of the nuclear reaction are suppressed[11] (a similar picture takes place also for the γ quanta[17]). However, for the described situation it is very important that particles of relatively low energy were involved, whereas now we are interested precisely in the motion of high-energy particles, with $\lambda \ll a$.

Let us consider now Eq. (3.1). It is easily seen that the modification of the ψ-function of the particle will be significant only if the coefficients

$$\frac{\overline{V}_\mathbf{K}}{E_{\mathbf{q}+\mathbf{K}}-E_\mathbf{q}}=2M\,\frac{\overline{V}_\mathbf{K}}{K^2+2\mathbf{q}\mathbf{K}} \tag{3.2}$$

are of appreciable magnitude.

For concreteness, we shall consider fast protons. Then, if we use (2.11) with

$$V_{\mathbf{K},j}=\frac{4\pi e^2}{K^2}[Z_j-F_j(\mathbf{K})] \tag{3.3}$$

($F_j(K)$ is the usual atomic form factor[18]), then for protons with energy of several MeV at an arbitrary direction g, the coefficients (3.2) turn out to be small even when $K = K_{min}$ (of the order of 10^{-2}).

It may seem at first glance that since $\overline{V}_K \sim 1/K^2$ at large values of K, and the denominator of (3.2) behaves like K in a wide range of K, a modification of the ψ-functions takes place and is manifest in the appearance of a large number of weakly perturbed waves with large K. This, however, is incorrect, since the presence of the exponential factor in (2.11) as a result of the oscillations of the atoms in the crystal causes the series in terms of "K" to converge rapidly. (We note that this circumstance is common to all dynamic problems in a crystal.)

Thus, at arbitrary g, no significant modification of the ψ function takes place, and this function is close to a plane wave, i.e., there is practically no collectivization.

However, for rigorously defined directions of q, namely, when q is close to the condition

$$\mathbf{q}\perp\mathbf{K}, \tag{3.4}$$

the picture changes radically. Indeed, the coefficients (3.2) cease in this case to depend on the particle energy. If it is recognized that $\overline{V}K_{min} \gg K^2_{min}/2M$, then it can be readily understood that in this case the coefficients (3.2) are large for an entire aggregate of reciprocal-lattice vectors, and collectivization therefore sets in.

The condition (3.4) is satisfied simultaneously for a one-dimensional chain of reciprocal-lattice vectors. This chain corresponds to a family of crystallographic planes perpendicular to it. Therefore the condition (3.4) corresponds to a motion of particles parallel to this family of crystallographic planes ("planar" channeling).

We emphasize that we assume at all times that the condition

$$M\overline{V}_{\mathbf{K}_{min}}/qK_{min}\ll 1 \tag{3.5}$$

is satisfied. Then, even the deviation of the wave vector of the particle from the separated chain K by only an amount equal to the vector K_{min} in the perpendicular direction leads to the appearance in (3.1) of terms known to be small (with the exception of the case when q is perpendicular to the plane of the reciprocal-lattice vector—see below). Therefore it is necessary to retain in this case in (3.1) the summation over only the one-dimensional chain of vectors K, for which the condition (3.4) is satisfied. If we designate the direction of this chain by x, then it follows from (3.1) that the problem reduces in this case to motion in a one-dimensional periodic potential, that depends only on x (see (2.11)),

$$V_{eff}(x)=\sum_{K_x}\overline{V}_{K_x}e^{iK_x x} \tag{3.6}$$

(the summation is carried out here over the discrete aggregate of the wave vectors of the selected one-dimensional chain).

The proper wave functions of the particle in such a potential, and the corresponding eigenvalues, take the form

$$\psi_{\mathbf{q},n}(\mathbf{r}) = e^{i\mathbf{qr}} \underset{K_x}{} \psi_{q_x+K_x,n} e^{iK_x x} \equiv e^{i\mathbf{qr}} U_{q_x,n}(x), \qquad (3.7)$$

$$E_{\mathbf{q},\,n} = (q_y{}^2 + q_z{}^2)/2M + \varepsilon_{q_x},\ n \qquad (3.7')$$

The index n (the number of the "band") label the states obtained by solving the system (3.1) with a one-dimensional potential (3.6).

In the general case, the entire set of coefficients $\psi_{q_x+K_x,n}$ in (3.7) will have comparable values. We thus arrive at an essentially one-dimensional collectivization of the transverse motion of the particles. The motion in the other two directions remains free.

We note that the larger the period along the chain K, i.e., the smaller the distance d between the crystallographic planes, the smaller the corresponding $\overline{V}_{K_x}$. It follows therefore that the collectivization becomes most strongly pronounced when the particles move along planes with minimal indices.

An important particular case of satisfaction of the condition (3.4) is motion along a direction perpendicular to the plane of the reciprocal-lattice vectors. This direction must be parallel to a certain chain of atoms in the crystal ("axial" channeling). Now the coefficients (3.2) are already important for a two-dimensional aggregate of reciprocal-lattice vectors, and we must retain the summation over them in (3.1). As a result we arrive at the motion of the particle in an effective two-dimensional periodic potential, defined in a plane parallel to the preferred plane of the reciprocal-lattice vectors (the summation is carried out over a discrete set of reciprocal-lattice points in this plane):

$$V_{eff}(\rho) = \sum_{\mathbf{K}_\perp} \overline{V}_{\mathbf{K}_\perp} e^{i\mathbf{K}_\perp\rho}. \qquad (3.8)$$

For the wave eigenfunctions of the particle and the energy eigenvalues we then obtain

$$\psi_{\mathbf{q},n}(\mathbf{r}) = e^{i\mathbf{qr}} \sum_{\mathbf{K}_\perp} \psi_{\mathbf{q}_\perp+\mathbf{K}_\perp,n} e^{i\mathbf{K}_\perp\rho} \equiv e^{i\mathbf{qr}} U_{\mathbf{q}_\perp,n}(\rho), \qquad (3.9)$$

$$E_{\mathbf{q},n} = q^2{}_z/2M + \varepsilon_{\mathbf{q}_\perp,n} \qquad (3.9')$$

($q_\perp$ is the projection of q on the preferred wave-vector plane and $q_z^2 = q^2 - q_\perp^2$).

The collectivization now has a two-dimensional character. It becomes all the more strongly manifest, the smaller the indices of the crystal chain along which the particle moves, and therefore the smaller the periods of the network of reciprocal-lattice points over which the summation is carried out in (3.8) and (3.9).

It is interesting that to determine the effective potentials (3.6) and (3.8) it suffices to know only the atomic form factor F as a function of the momentum transfer (see (3.3)). This is all the more important, since F can be regarded as a known quantity either on the basis of the experimental results (for example, from the scattering of x-rays), or on the basis of the use of known approximate theoretical results.

A few general remarks concerning the character of the behavior of the effective potential. If the unit cell of the crystal contains only one atom, then the effective potential turns out to be maximal on the crystallographic planes of the preferred family in the case of (3.6) and at the points of intersection of the preferred family of atomic chain with the plane on which the potential is defined in the case of (3.8). It is significant that in both cases the potential has inversion with respect to the points where it reaches a maximum. If the unit cell contains more than one atom, then in the general case the potential has several maxima and does not have the inversion of the type indicated above.

Another important circumstance is that the effective potential decreases with increasing temperature owing to the increase of the probability of the excitation of the phonons, and consequently owing to the decrease of the probability of the purely elastic scattering of the particles in the oscillating crystal. It is important that different Fourier components of the potential vary with temperature differently. The Fourier components that decrease foremost with the temperature are those with large K. This is the reason for the change in the form of the effective potential with temperature, and the potential changes most noticeably, as a rule, in the region of its maximum values, just where the contribution of the Fourier component with large K is important.

All these statements can be clearly traced in Fig. 1, which shows, for purposes of illustration, the one-dimensional effective potentials, $V_{eff}(x)$ for germanium and silicon at several directions of K and several values of the temperature. The Z(q) (2.9) were calculated in the Debye approximation with standard values of the Debye temperatures, 296 and 543°K respectively for germanium and silicon. The parameters of the crystal lattices were taken from[19], and the Moliere approximation for the potential of the interaction between the proton and the individual atom[20] was used in the determination of $\overline{V}_K$.

For potentials of the type shown in the figures, the motion of protons with energy $\epsilon < V_{eff}^{max}$ will have a predominantly quasiclassical character. The quantum effects come into play principally for states with transverse-motion energy near the top of the barrier. As will be seen from now on, the character of motion of the particles in this energy region is very important for the phenomena of interest to us. Therefore, in particular, the temperature modification of the potential near its maximum value is also important.

4. PLANAR CHANNELING

In this paper we confine ourselves to an analysis of planar channeling. We consider a crystal in the form of a plate and assume for convenience that the input surface is perpendicular to a certain family of crystallographic planes. Let the particle flux be incident at a certain small angle $\vartheta = q_x/q$ to these planes (the normal to the plane is the x axis, and the normal to the input surface is the z axis). Then we select the system (3.7) as the complete system of functions for the determination of the density matrix. We note here that in determining the complete set of functions we can use both the value of $\tilde{q}_x$ referred to the first cell of the

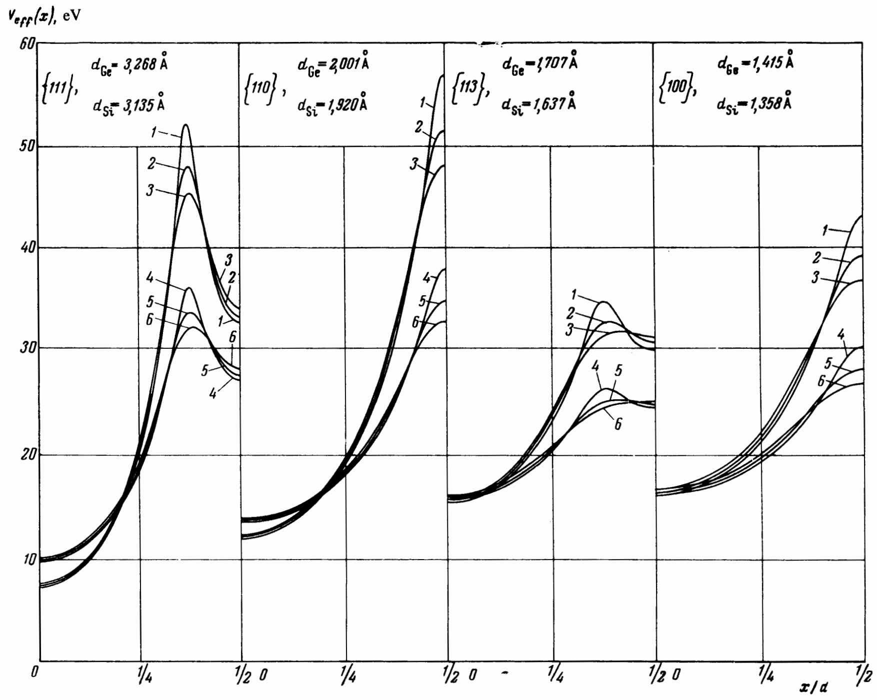

FIG. 1. $V_{eff}(x)$ for certain crystallographic planes in germanium and silicon. Curves 1, 2, and 3 were constructed for germanium at temperatures 0, 300, and 590°K respectively, and curves 4, 5, and 6 for silicon at 0, 540, and 1090°K. The point x = 0 corresponds to the absolute minimum of the potential and, just like the point x = d/2, is an inversion center of $V_{eff}(x)$.

reciprocal lattice,

$$q_x = \tilde{q}_x + \tilde{K}_x, \tag{4.1}$$

and simply the "total" value of q_x, taking into account the corresponding conditions for the Bloch functions and energy:

$$U_{q_x+K_x,n}(x) = e^{-iK_x x} U_{q_x,n}(x), \quad \varepsilon_{q_x+K_x,n} = s_{q_x,n}. \tag{4.2}$$

We shall assume that the index $s_1 \equiv \{\tilde{q}_{1x}, q_{1y}, q_z n_1\}$. The initial values of the density matrix in this representation will be determined by the expression (2.13) with

$$C_{s_1}(\mathbf{q}) = \delta_{q_y q_{1y}} \delta_{q_z, q_{1z}} \sum_{K_x} \delta_{q_x - \tilde{q}_{1x}, K_x} \psi_{q_x, n_1}{}^{*}. \tag{4.3}$$

We confine oursevelves here to sufficiently thin crystals, to be able to neglect the elastic scattering of the particles. We shall not stop to define the appropriate criterion, which will be considered in detail in a subsequent paper, devoted especially to the role of inelastic processes in channeling.

In the absence of inelastic processes, the solution of (2.3) takes the form

$$\rho_{1s_1s_2}(t) = \rho_{1s_1s_2}(0) \exp\{-i(E_{s_1} - E_{s_2})t\}. \tag{4.4}$$

Substituting this solution in (2.14) and taking (2.13), (4.3), and (4.2) into account, we obtain for the density of the particles in the crystal

$$n_{q_x}(x,t) = \sum_{n_1 n_2} \psi_{q_x n_1} \psi_{q_x, n_2} U_{q_x, n_1}(x) U^{*}_{q_x, n_2}(x) \times \exp\{-i(\varepsilon_{q_x, n_1} - \varepsilon_{q_x, n_2})t\}. \tag{4.5}$$

This expression contains in main outline already the entire channeling picture. Indeed, at t = 0 the nondiagonal elements of the density matrix are strictly correlated with each other, leading, as can be readily shown, to the fact that $n_{q_x}(x, 0)$ = const. In other words, the particle density is uniform, as it should be. However, on moving inside the crystal, the relation between the non-diagonal elements $\hat{\rho}_1$(4.4) changes, meaning the appearance of a density distribution that is not uniform in x. To see how radically this distribution changes, we obtain the value of the density averaged over the thickness of the crystal:

$$n_{q_x}(x) = \sum_n |\psi_{q_x, n}|^2 |U_{q_x, n}(x)|^2. \tag{4.6}$$

We analyze this expression, taking into account the fact that

$$\sum_n \psi^{*}_{q_x, n} \psi_{q_x+K_x, n} = \delta_{0, K_x}. \tag{4.7}$$

When $\epsilon_{q_x}, n < V_{eff}^{max}$, the penetration through the barrier will turn out to be very weak for those effective-potential parameters which should obtain in real crystals (see the preceding section). Therefore the motion along the x axis has a quasiclassical character, and the ψ-functions at different values of n have an oscillating behavior characterized, roughly speaking, by a certain characteristic momentum of the particle. A sufficiently large number of "bands" fits in the resultant "well," and most of these bands have a weak dispersion (weak dependence on $\tilde{q}_x$). By virtue of the foregoing, the expression (see (4.1) and (4.2))

$$\psi_{q_x, \tilde{n}} = \frac{1}{d} \int_0^d U_{q_x, n}(x)\, dx = \frac{1}{d} \int_0^d \exp\{-i\tilde{K}_x x\} U_{\tilde{q}_x, n}(x)\, dx \tag{4.8}$$

will have a noticeable value only for those n for which the characteristic momentum of the particle is close to $\tilde{K}_x$ and (the energy is reckoned from the bottom of the well).

$$\varepsilon_{q_x, n} \approx \tilde{K}_x^2 / 2M.$$

Thus, specifying a definite angle of incidence ϑ (a definite q_x) is equivalent to defining a certain narrow interval of n, within which the particle is localized. However, there is still one more interval of n where (4.8) differs appreciably from zero at $\tilde{K}_x^2/2M$

$< V_{\mathrm{eff}}^{\max}$. We have in mind the above-the-barrier states, for which the corresponding momentum is

$$[2M(\varepsilon_{q_x,n} - V_{eff})]^{1/2} \sim |\tilde{K}_x|. \qquad (4.9)$$

These states play a very important role, since, in accordance with the usual quasiclassical form of the wave function[18]

$$\psi(x) = \frac{c_1}{\sqrt{p_x}} \exp\left\{ i \int p_x \, dx \right\} + \frac{c_2}{\sqrt{p_x}} \exp\left\{ -i \int p_x \, dx \right\}, \qquad (4.10)$$

the particle "hovers" a long time over the barrier in such states, producing a high particle density precisely at the locations of the nuclei.

If we ignore, at small particle incidence angles, the existence of above-the-barrier states, then in accordance with (4.6) and (4.7) the particle distribution density averaged over the thickness will decrease exponentially towards the region of the equilibrium position of the nuclei, as a result of the above-the-barrier behavior of $E_{q_x,n}(x)$. In the absence of oscillations of the nuclei, this leads to the vanishing of the nuclear reaction, of large-angle scattering, of ionization from the internal shells, etc. In this sense, we arrive at a clear cut channeling effect, and the limiting angle of incidence for which this picture is still valid—the channeling angle ϑ_0—is determined simply as (we assume for simplicity a potential with a single maximum)

$$\vartheta_0(T) \approx \frac{\sqrt{2MV_{eff}^{\max}(T)}}{q} = \frac{q_x^*}{q} \qquad (4.11)$$

(T is the crystal temperature).

This angle, however, has an arbitrary character, for even when $\vartheta \ll \vartheta_0$ an important role is played in (4.6) and (4.7) by above-the-barrier states with the aforementioned behavior singularity, and the particle density in the region of location of the nuclei, while relatively small, remains finite. We note also that on approaching the top of the barrier, tunneling of particles, which leads to an effective decrease of ϑ_0 may become significant.

When $\vartheta \gtrsim \vartheta_0$ the main density of states is connected with a narrow interval of states that are directly adjacent in energy to the top of the barrier. In connection with the character of the behavior of the quasiclassical function (4.10) in this region, and with the aforementioned "hovering" effect, the density of the particles $n_{q_x}(x)$ near the nuclei should increase in this case sharply compared with the value averaged over x. As a result, the yield of the nuclear reaction at such particle-incidence angles should be noticeably higher than in the usual non-channeling motion of the particles.

Since we intend to trace in succession all the results, we have considered the solution of the problem for a model potential $V_{eff}(x)$ in the form of the well known Kronig-Penney potential with height V_0, width b, and period d. Knowing the forms of the eigenfunctions and the eigenvalues for such a potential, and determining $\psi_{q,n}$ [Eq. (4.8)], we can find all the quantities of interest to us by using a computer for this purpose.

Figure 2 shows plots of the nuclear reaction yield $\overline{I}(q_x)$ averaged over the thickness (in relative units) as functions of the incident wave vector q_x. In an oscillating crystal, the intensity of the nuclear reaction at the nucleus of type j is connected with the particle density (4.5) by the average relation

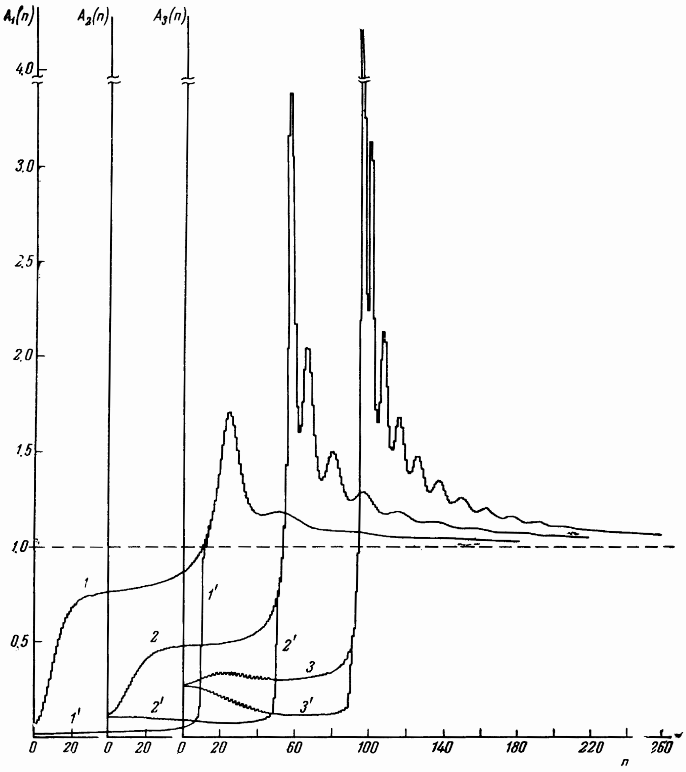

FIG. 2. Yield of nuclear reaction $A(n) \equiv I(K_x^0(n + 1/2)/2)$ averaged over the thickness, for different values of the parameter b of the Kronig-Penney potential: 1 – 0.04 Å, 2 – 0.08 Å, 3 – 0.12 Å.

$$I(q_x, t) = \sum_{K_x} n_{q_x}(K_x, t) e^{iK_x x_j} e^{-Z_j(K_x)/2} = \int_{-\infty}^{\infty} n_{q_x}(x, t) W_j(x) \, dx, \qquad (4.12)$$

where $n_{q_x}(K_x, t)$ is the Fourier component of the quantity $n_{q_x}(x, t)$, and $W_j(x)$ is given by

$$W_j(x) = \frac{1}{\sqrt{2\pi u_{T,j}^2}} \exp\left\{ -\frac{(x - x_j)^2}{2u_{T,j}^2} \right\} \qquad (4.12')$$

($u_{T,j}^2$ is the mean square of the thermal displacement of the j-th atom from the equilibrium position along the x axis). The figure therefore shows the values of (4.6) after an averaging of the type (4.12). The calculations were performed at three values of the parameter b equal to 0.04, 0.08, and 0.12 Å. The values of the other parameters approximately coincided with the corresponding characteristics of the {110} plane channel in germanium at T = 0°K and were equal to

$$d = 2\,\text{Å}, \quad d\sqrt{2MV_0} = 300, \quad u_T = 0.04\,\text{Å}. \qquad (4.13)$$

We note that the true value of the barrier width at $\epsilon_{q_x,n} \ll V_{\mathrm{eff}}^{\max}$ does not play a major role. To the contrary, the width of the barrier near the top is very important for the entire picture of the phenomenon. Therefore the barrier widths in the calculations were chosen to lie in the interval close to the real interval precisely for the top part of the barrier.

The curves shown in Fig. 2 duplicate very clearly both all of the qualitative features of the phenomenon, which were determined above, and the experimentally observed picture of the effect. A sharp dip is seen and the channeling angle is clearly pronounced. $\bar{I}(q_x)$, however, never reaches zero at $\vartheta < \vartheta_0$, this being connected with the role of the above-the-barrier states and with the oscillations of the nuclei (the dip at $\vartheta < \vartheta_0$ decreases with increasing temperature). The curves 1′, 2′, 3′ contribute to the corresponding values of $\bar{I}(q_x)$ of the above-the-barrier and of the five highest below-the-barrier bands. We see that with increasing barrier thickness the contribution of these states to $\bar{I}(q_x)$ increases when q_x is close to zero. For abscissas larger than 100, the primed curves practically coincide with the unprimed ones. Above the angle ϑ_0, the yield of the reaction is much higher than the mean yield ($\bar{I} = 1$), and the decrease towards the mean value is relatively slow. Thus, both the channeling itself and the role of the above-the-barrier states become very clearly manifest. At such a character of the channeling, the inelastic processes will be strongly suppressed at $\vartheta < \vartheta_0$. Therefore, for this region of angles, the length over which the inelastic processes play an unimportant role greatly increases.

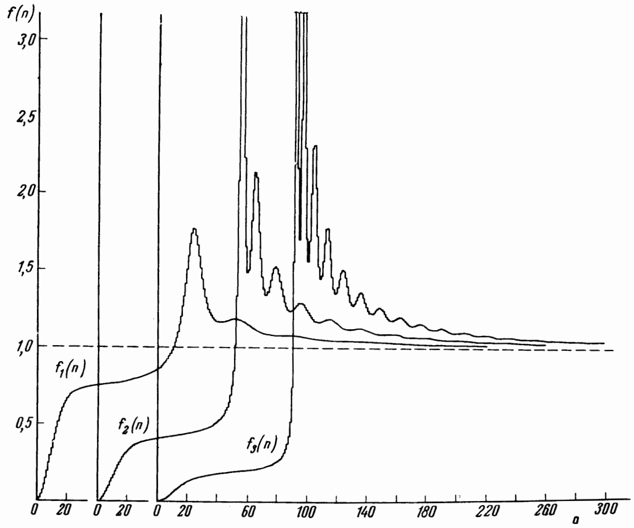

FIG. 3. Thermal mean value $f(n) \equiv \langle |U_{K_x^0/4,\,n}|^2 \rangle$ on the nucleus as a function of the band number n: f_1 – at b = 0.04 Å, f_2 – b = 0.08 Å, f_3 – b = 0.12 Å. The values of the functions are: $f_2(95) = 3.761$, $f_2(96) = 5.165$, $f_2(97) = 3.711$; $f_3(92) = 6.532$, $f_3(93) = 7.166$, $f_3(97) = 3.582$, $f_3(98) = 3.419$.

It is interesting that $\bar{I}$ as a function of ϑ has an oscillatory structure (the corresponding angle periods are small, and to observe the angles it is necessary to have a beam collimation much higher than the existing one). These are typically quantum oscillations of the yield of the nuclear reaction, and are the results of the oscillations in the yield from the closer quantum levels. This is clearly seen in Fig. 3, which shows plots against n of the thermal mean values $\langle |U_{K_x^0/4,n}|^2 \rangle$ on the nucleus ($K_x^0 = 2\pi/d$ is the elementary reciprocal-lattice vector), for the same Kronig-Penney potential as in Fig. 2((unity is chosen to be the corresponding value in the case of plane waves). The value b = 0.04 Å corresponds to 94 sub-barrier bands, for b = 0.08 Å the number of such bands is 92, and for b = 0.12 Å the number is 90. The oscillations of the curves in the regions of n corresponding to the above-the-barrier bands have a quantum nature and are governed by whether a maximum or a minimum of the function $|U_{K_x^0/4,n}(x)|^2$ falls in the small vicinity of the equilibrium coordinate of the nucleus. The curves demonstrate, in particular, the increase in the role of the thermal oscillations of the nuclei with increasing thickness of the potential barrier.

We note that there exists a unique analogy between the oscillations of the quantity $\bar{I}(q_x)$ and the known quantum oscillations of the different physical quantities

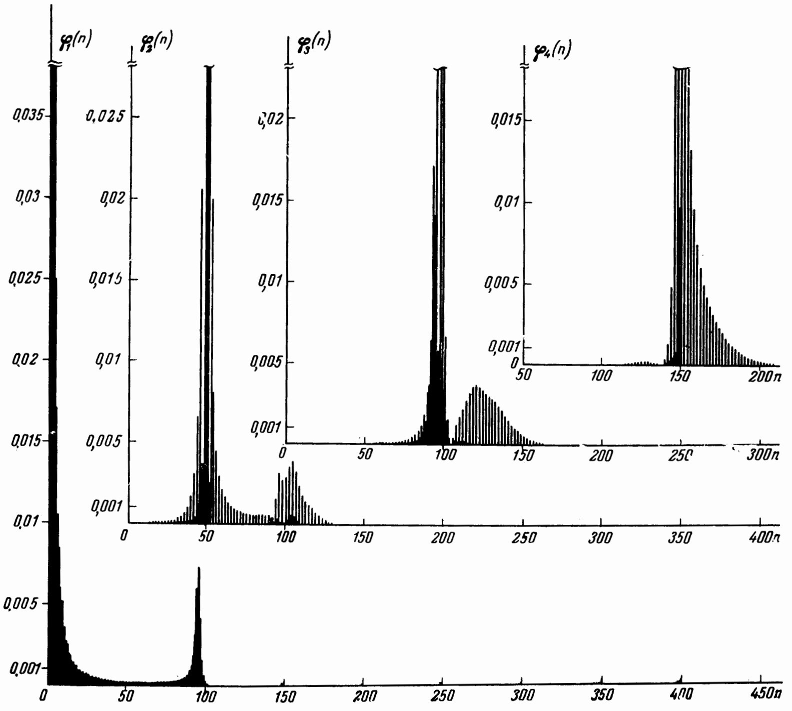

FIG. 4. Population of the energy bands $\varphi(n) \equiv |\psi_{q,n}|^2$ in a Kronig-Penney potential with b = 0.08 Å. The functions $\varphi_1(n)$, $\varphi_2(n)$, $\varphi_3(n)$, and $\varphi_4(n)$ correspond to q_x equal to $0.25K_x^0$, $25.25K_x^0$, $49.25K_x^0$, and $75.25K_x^0$. We have here $\varphi_1(1) = 0.7020$, $\varphi_1(2) = 0.1047$, $\varphi_1(3) = 0.04833$; $\varphi_2(48) = 0.2556$, $\varphi_2(49) = 0.4736$, $\varphi_2(50) = 0.1403$; $\varphi_3(95) = 0.3821$, $\varphi_3(97) = 0.4580$, $\varphi_3(99) = 0.02915$; $\varphi_4(147) = 0.02455$, $\varphi_4(149) = 0.6380$, $\varphi_4(151) = 0.1872$, $\varphi_4(153) = 0.04110$, $\varphi_1(155) = 0.02054$.

in a metal in a magnetic field. There, too, the electron is characterized by a quasiclassical motion with a quantum number amounting to several times 10. The necessary accuracy of the angular collimation corresponds here to the accuracy with which the magnetic field is fixed there. For both cases, the inelastic processes for the particles smear out the oscillations.

In order to determine the character of the band population as a function of the particle incidence angle, Fig. 4 shows plots of $|\psi_{q,n}|^2$ against n for four values of q_x, corresponding to values of ϑ close to 0, $\vartheta_0/2$, ϑ_0, and $3\vartheta_0/2$, in a Kronig-Penney potential with b = 0.08 Å. We see that the picture is close to that qualitatively formulated above.

So far we have carried out the entire analysis for quantities averaged over the thickness of the crystal. We now turn to the initial equation for the particle density $n_{q_x}(x, t)$ (4.5). The energy difference which enters in the phases of (4.5) will have a minimum value for the nearest bands

$$\varepsilon_{q_x,n+1} - \varepsilon_{q_x,n} \approx q_x K_x^0/M.$$

The value of the phase after the particle traverses a thickness l is

$$(\varepsilon_{q_x,n+1} - \varepsilon_{q_x,n})t \approx 2\pi \frac{q_x}{q}\frac{l}{d}. \qquad (4.14)$$

It follows therefore that the complete "averaging out" of all the phases for the angle region $\vartheta \ll \vartheta_0$ of interest to us occurs under the condition

$$l/d \gg 1/\vartheta_0. \qquad (4.15)$$

However, the principal realignment of the state of the particle from a plane wave to a collective state, corresponding to a sharp change of the density near the location of the nucleus, occurs at much smaller distances. The point is that if we expand the plane wave in terms of the states (3.7), then the homogeneous density in x arises only as a result of a clear cut phase relation between the above-the-barrier and below-the-barrier states. But these phases become mismatched at much smaller distances than (4.15). Indeed, let $\vartheta \ll \vartheta_0$. Then the minimum phase difference between the above-the-barrier and below-the-barrier states is of the order of (see (4.11) for a definition of q_x^*)

$$V_{eff}^{\max} t \approx \pi\vartheta_0 \frac{q_x^*}{K_x^0}\frac{l}{d}. \qquad (4.16)$$

It follows therefore that the characteristic distance l_1, over which the mismatch of these phases takes place, is

$$\frac{l_1}{d} \approx \frac{K_x^0}{q_x^*}\frac{1}{\vartheta_0}. \qquad (4.17)$$

Allowance for the oscillations of the atoms causes an appreciable change in the role of the nuclear reaction and in the scattering through large angles to occur over distances cl_1 from the input surface, where c is a constant ranging from several units to several times 10, depending on the width of the barrier in the Kronig-Penney potential. At a fixed temperature, the constant c turns out to be the smaller, the smaller the width of the barrier. This is connected with the fact that when the width of the barrier decreases the nucleus has a larger probability of being located in regions near the potential walls, while the ψ-function of the particle becomes most strongly modified (over distances on the order of l_1).

In connection with the described picture of the phase mismatch, there should exist a very unique effect, recalling phenomena of the "echo" type. Let $\vartheta \ll \vartheta_0$. Then, as we have already noted, the spectral density of the states becomes localized in narrow intervals near the bottom of the well and near the top of the barrier. It is easy to see that the density of the particles in the small region near the position of the equilibrium of the nucleus is produced principally as a result of above-the-barrier states. On moving to the interior of the crystal, a mismatch of the phases of these states sets in. However, at a certain thickness l_0 on the order of

$$l_0/d \sim 1/\vartheta_0 \qquad (4.18)$$

the phase difference corresponding to the main and

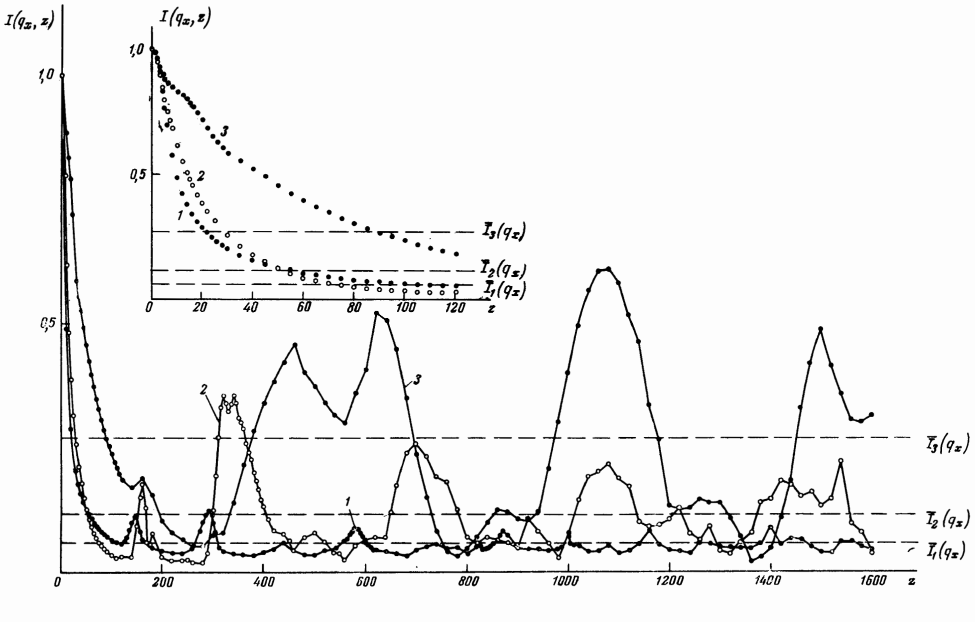

FIG. 5. Yield of the nuclear reaction I(q_x, z) (in relative units) as a function of the coordinate of the nucleus z for $q_x = (1/4)K_x^0$. Here z is measured in units of q_z/MV_0. Curves 1–3 correspond to the same values of the parameter b as in Fig. 2.

above-the-barrier distributions of the states becomes close to 2π. This leads to a spike in the yield of the nuclear reaction. Such an "echo" can be repeated in principle several times with changing distance from the surface. Thus, a typical size effect is produced.

Of course, the exact value of l_0 depends on the character of the above-the-barrier energy spectrum and on its population.

The described picture of the phenomenon is very distinctly traced in an analysis carried out for a concrete model of the effective potential. Figure 5 shows plots of I as functions of the running thickness z(t) in an oscillating crystal with the same characteristics (4.13) of the planar channel and with the values of the parameter b used in the calculations of the curves of Figs. 2 and 3.

As to the angular distribution of the particles, by substituting (4.4) in (2.17) and taking (2.13), (4.3), and (4.2) into account, we get

$$\rho_1(\varkappa, t) = \delta_{\varkappa_y, q_y} \delta_{\varkappa_z, q_z} \sum_{K_x} \delta_{\varkappa_x - q_x, K_x} \times \Big| \sum_n \psi^*_{q_x, n} \psi_{\varkappa_x, n} \exp\{-i\varepsilon_{q_x, n} t\} \Big|^2. \tag{4.19}$$

When t = 0, taking (4.7) into account, we get

$$\rho_1(\varkappa, 0) = \delta_{\varkappa_x, q_x} \delta_{\varkappa_y, q_y} \delta_{\varkappa_z, q_z}, \tag{4.20}$$

i.e., as expected, it is only an incident plane wave on the input surface.

With increasing t, i.e., as the particle moves to the interior of the crystal, discrete beams are produced, which are diffracted relative to the incident beam by the vectors K_X. To ascertain which of them can be most strongly represented, let us examine the values $\rho_1(\kappa)$ of (4.19), averaged over the thickness of the crystal:

$$\bar{\rho}_1(\varkappa) = \delta_{\varkappa_y, q_y} \delta_{\varkappa_z, q_z} \sum_{K_x} \delta_{\varkappa_x - q_x, K_x} \sum_n |\psi_{q_x, n}|^2 |\psi_{\varkappa_x, n}|^2. \tag{4.21}$$

Let $\vartheta < \vartheta_0$. Then, starting from the character of the population of the low-lying energy bands and from the behavior of the corresponding eigenfunctions, we can easily see that in expression (4.21), besides the κ_X that are "close" to q_X, there will also be represented beams with κ_X "close" to $-q_X$. This means that as the particle penetrates to the interior of the crystal a "specular" reflection of the particles takes place from the considered crystallographic planes.

In addition, since at such incidence angles the population of the above-the-barrier bands becomes significant, beams scattered through angles on the order of the channeling angle ϑ_0 will be relatively noticeably represented in (4.21).

Numerical estimates and concrete calculations show that the "specularly" reflected beams acquire their intensity at distances l_2 on the order of

$$l_2 / d \approx q / q_x \tag{4.22}$$

(at $\vartheta = 0$ the quantity q_X in this estimate is replaced by K_X^0). With further increase of z(t), in close correspondence with the classical picture of the phenomenon, a periodic redistribution of the intensity takes place between the "specularly" reflected beams (i.e., between beams with κ_n close to q_X and beams with κ_X close to $-q_X$) with a period $2l_2$.

As to the beams scattered through angles on the order of ϑ_0, the appearance of which is due to above-the-barrier states, their intensity is established at distances from the input surface much smaller than l_2, causing by the same token a rapid modification of the state of the particle, particularly a sharp decrease of the particle density at the nuclear of the crystal with the distance.

The authors are most grateful to A. M. Afanas'ev for valuable discussion and to M. Ya. Omelik for help with the computer calculations.

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Translated by J. G. Adashko
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