

KINETICS OF CHANNELING WITH RECHANNELING

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Побудована система рівнянь кінетичної теорії каналювання з обліком реканалювання. Отримано нові вираження для функції деканалювання враховуючі можливість деканалювання, об'ємного захоплення і реканалювання на жорстких дефектах. Показано існування нових характерних довжин у кінетиці каналювання – це довжини реканалювання й об'ємного захоплення. Також показано, що облік розподілу часток по поперечним перемінним приводить до модифікації ертуру деканалювання на дефектах.

Построена система уравнений кинетической теории каналирования с учетом реканалирования. Получены новые выражения для функции деканалирования учитывающие возможность деканалирования, объемного захвата и реканалирования на жестких дефектах. Показано существование новых характерных длин в кинетике каналирования – это длины реканалирования и объемного захвата. Также показано, что учет распределения частиц по поперечным переменным приводит к модификации сечения деканалирования на дефектах.

The basic system of equations of the kinetic theory of channeling with rechanneling is built. A new expression is obtained for channeled fraction taking into account the volume trapping, and rechanneling and dechanneling on rough defects. The existence of new characteristic lengths - the volume trapping length and the rechanneling length - is shown. It is shown, that flux peaking effect modifies the dechanneling cross-sections of the defects.

It is well known that volume trapping of chaotically moving particles in the channeling regime (rechanneling) plays a considerable role in directional effects. However, as yet there is no kinetic theory in which these processes would be included for consideration. In this paper the basis of such a theory is built and principal properties of channeling processes with rechanneling are discussed. The work is the development of the theory of dechanneling presented earlier [1].

In order to include the trapping effects in consideration one must study two fractions of particles moving in crystal - random and channeled. Moreover the random fraction may also be subdivided into two fractions, namely, the particles that begin their motion in crystal in chaotic regime, and dechanneled particles. This subdivision follows from simple physical considerations: the state of initially random fraction strongly depends on the initial conditions of particles penetration into the crystal, but there is no such dependence for the dechanneled fraction. Then we must also separate the process of volume trapping of initially non-channeled particles in channeling and the process of rechanneling. The same reason may be required to divide channeled particles into two fractions too: the initially channeled particles and particles trapped into the channeled motion. Therefore, for complete kinetic description of the directional phenomena we must introduce four distribution functions: the distribution function of initially random fraction of particles $F_r^p(x, z)$, the initially channeled particle distribution function $F_c^p(x, z)$, the rechanneled particle distribution

function $F_c^s(x, z)$ and the dechanneled particle distribution function $F_r^s(x, z)$. In our notation z is the penetration depth along one of close-packed axes or planes in crystal and the vector x represents the set of variables (coordinates and velocities), which describes the motion of particles transverse to this axis or plane. These distribution functions will satisfy four related kinetic equations.

Let us discuss now the type of these equations. It depends directly on the origin of the forces acting on particles moving in the crystal. It is good known, that particles experience in crystal the forces caused by potential of the channel (channeled fraction), the damping caused by interaction with electrons, the random small-angle scattering on thermally vibrating crystal atoms and electrons and rare random large-angle scattering on crystal atoms and defects. Therefore, there are two main mechanisms of change of the particle transverse motion state: the diffusion and rare dramatic its change due to close impacts with crystal atoms and different crystal defects. After it these equations will be the equations of the Chapman-Kolmogoroff type, and the connection between them is realized by collision integrals in their right-hand sides. In the general case, these equations may be written as

$$\frac{\partial F_c^p(z, \vec{x})}{\partial z} + L_{ch}\{F_c^p(z, \vec{x})\} = - \sum_i I_{c \rightarrow r}^i; \quad (1)$$

$$\frac{\partial F_c^s(z, \vec{x})}{\partial z} + L_{ch}\{F_c^s(z, \vec{x})\} = - \sum_i (I_{c \rightarrow r}^i - I_{r \rightarrow c}^i); \quad (2)$$

$$\frac{\partial F_r^p(z, \vec{x})}{\partial z} + L_r\{F_r^p(z, \vec{x})\} = - \sum_i I_{r \rightarrow c}^{*i} + I_r^{*p}; \quad (3)$$

$$\frac{\partial F_r^s(z, x)}{\partial z} + L_r \{F_r^s(z, \vec{x})\} = - \sum_i (I_{r \rightarrow c}^{*i} - I_{c \rightarrow r}^{*i}) + I_c^* + I_r^*$$

(4) where L_{ch} is the Fokker-Plank operator over the variables x for the channeled fraction, L_r is the diffusion type operator over the variables x for the disordered fraction, and $I_{c \rightarrow r}^i$, $I_{c \rightarrow r}^{*i}$, $I_{r \rightarrow c}^i$, $I_{r \rightarrow c}^{*i}$ are the collision integrals describing transitions of particles between initially random (r) and channeled (c) states due to various mechanisms. They may be represented in the following forms

$$I_{r \rightarrow c}^i = \int_V dx' F_r^{p,s}(z, \vec{x}') \cdot w_i(z, \vec{x}' \rightarrow \vec{x}) ; \quad (5)$$

$$I_{r \rightarrow c}^{*i} = \int_V dx' F_r^{p,s}(z, \vec{x}) \cdot w_i(z, \vec{x} \rightarrow \vec{x}') ; \quad (6)$$

$$I_{c \rightarrow r}^i = \int_V dx' F_c^{p,s}(z, \vec{x}) \cdot w_i(z, \vec{x} \rightarrow \vec{x}') ; \quad (7)$$

$$I_{c \rightarrow r}^{*i} = \int_V dx' F_c^{p,s}(z, \vec{x}') \cdot w_i(z, \vec{x}' \rightarrow \vec{x}) . \quad (8)$$

The right-hand side of equation (4) also contains the collision integral $I_{c \rightarrow r}^*$, which describes the dechanneling due to slow diffusion-type increase in the transverse energy E_{\perp} of channeled particles and subsequent their large-angle scattering on the atoms of atomic chains or planes when this energy becomes equal to its critical value $E_{\perp c}$ and the reflection randomly moved particles from the boundary of channel due to blocking effect:

$$I_c^* = \varphi(x, z) \cdot [J_c(x, F_c(z, \vec{x}))]_{x \in S}^- ; \quad (9)$$

$$I_r^{(p,s)*} = \varphi(x, z) \cdot [J_r(x, F_r^{p,s}(z, \vec{x}))]_{x \in S}^- , \quad (10)$$

where

$$L_{ch,r}(F_{c,r}(z, \vec{x})) = \frac{\partial}{\partial x} J_{c,r}(\vec{x}, F_{c,r}(z, \vec{x})) . \quad (11)$$

In formulas (5)-(11), V and V' are the phase volumes, which correspond to channeled and non-channeled states respectively, S are the boundary surface between V and V' (the surface S is defined by the equality $E_{\perp}(x) = E_{\perp c}$), $C_i(z, x)$ is the concentration of the rough defects of kind i in the channels, $\varphi(x, z)$ is the x distribution of the particles which have dechanneled within the penetration depth z , $w_i(z, x \rightarrow x')$ is the probability of the transitions of particles between states due to the i mechanism.

The initial conditions for distribution functions $F_c^{p,s}(z, x)$ and $F_r^{p,s}(z, x)$ by definition are:

$$F_c^s(0, \vec{x}) = F_r^s(0, \vec{x}) = 0 ; \quad (12)$$

$$F_c^p(0, \vec{x}) = \Lambda_{ch}^0(\vec{x}) ; \quad (13)$$

$$F_r^l(0, \vec{x}) = \Lambda_r^0(\vec{x}) . \quad (14)$$

The distribution functions $F_c^{p,s}(z, \vec{x})$ and $F_r^{p,s}(z, \vec{x})$ will also satisfy some boundary conditions on the surface S which separates the phase volumes V and V' . We shall not discuss these conditions here because our conclusions will not depend on their particular form.

Because initial value of rechanneled particle distribution function $F_c^s(x, z)$ and the dechanneled particle distribution function $F_r^s(x, z)$ always equals zero, it is possible to introduce joined channeled particles distribution function:

$$F_c(x, z) = F_c^p(x, z) + F_c^s(x, z) \quad (15)$$

and joined random moving particles distribution function:

$$F_r(x, z) = F_r^p(x, z) + F_r^s(x, z) . \quad (16)$$

The system (1)-(4) is the basic system of equations of the kinetic theory of channeling with rechanneling and volume trapping. We shall not give full analysis of this system here, but we shall use it in order to ascertain the principal properties of channeling with rechanneling. For this purpose let us construct the formal solution of sum of equations (1)-(2) for joined channeled particles distribution function, by expansion of it in the eigenfunctions of the operator L_{ch} with any given boundary conditions. Using then the results of [1] one can get the following general expression for the channeled fraction

$$P_c(z) = \int_V dx F_c(z, \vec{x}) = q \exp\left[-\frac{z}{R_{ch}}\right] + \int_0^z d\zeta \exp\left[-\frac{z-\zeta}{R_{ch}}\right] \left\{ \frac{P_r(\zeta)}{R_r(\zeta)} \right\} , \quad (17)$$

where

$$\begin{aligned} (R_{ch}^*)^{-1} &= \lambda + \sum_i \left[\frac{1}{z} \int_0^z dt \int_V dx \frac{F^2(x)}{\|F\|^2} \int_V dx' w_i(t, \vec{x} \rightarrow \vec{x}') \right] = \\ &= (R_{ch})^{-1} + \sum_i [R_{ch}^i(z)]^{-1} = (R_{ch})^{-1} + (R_{ch}^d)^{-1} ; \quad (18) \end{aligned}$$

$$\begin{aligned} R_r^{-1}(z) &= \int_V dx \int_V dx' \frac{F(x)F(x')}{\|F\|^2} * \\ &\left\{ \sum_i \int_{V'} dx'' \Phi_r(x'', z) \cdot w_i(z, \vec{x}'' \rightarrow \vec{x}') \right\} \quad (19) \end{aligned}$$

In formulas (17) - (19) the functions $P_r(z)$ and $\Phi_r(x, z)$ are defined by the equality

$$\begin{aligned} F_r(z, x) &= P_r(z) \Phi_r(x, z) = \\ &= P_r^p(z) \Phi_r^p(x, z) + P_r^s(z) \Phi_r^s(x, z), \quad (20) \end{aligned}$$

$R_{ch} = \lambda^{-1}$ is the dechanneling length in crystals without rough defects ("diffusion dechanneling length"), λ and $F(x)$ are respectively the first eigenvalue and the first eigenfunction of Fokker-Plank operator L_{ch} at given boundary conditions,

$$\|F\| = \left[\int_V dx F^2(x) \right]^{1/2} \text{ and } q = P_c(0) \text{ (see [1])} .$$

Let us discuss formula (17). First of all, it contains a well-known exponential term describing dechanneling process at the absence of rechanneling and volume trapping. There is a sole but essential distinction of this term from given earlier [1] expression for channeled fraction: in this terms the diffusion dechanneling length

$R_{ch} = \lambda^{-1}$ is replaced with a more general dechanneling length R_{ch}^* defined by formula (18). As it follows from this formula the presence of rough defects in crystals causes the existence, besides R_{ch} of the set of new dechanneling lengths $R_{ch}^i(z)$ each of them describes the dechanneling on the defects of one kind:

$$R_{ch}^i(z) = \left[\frac{1}{z} \int_0^z dt \int_V dx \frac{\vec{F}^2(x)}{\|F\|^2} \int_V dx' w_i(z, \vec{x} \rightarrow \vec{x}') \right]^{-1} \quad (21)$$

The probability of dechanneling on rough defect can be written as:

$$w_i(z, \vec{x} \rightarrow \vec{x}') = C_i(z, \vec{x}) \cdot \frac{d\sigma(\vec{x} \rightarrow \vec{x}')}{dx} \quad (22)$$

As one can see, these dechanneling lengths are the functions of penetration depth z if the rough defect concentrations C_i depend on z .

For almost all rough defects the dependence of concentrations C_i on x has a form:

$$C_i(z, x) = C_i(z) \delta(x - x_i), \quad (23)$$

where x_i are transverse positions of the defects i in the channels. Taking into account this fact one can write the exponential term in formula (12) in the form

$$q \exp\left[-\frac{z}{R_{ch}^*}\right] = q \exp\left[-\frac{z}{R_{ch}} - \sum_i \int_0^z dt C_i(t) \sigma_i\right], \quad (24)$$

where

$$\sigma_i = \frac{F^2(x_i)}{\|F\|^2} \int_V dx' \left[\frac{d\sigma_i(\vec{x} \rightarrow \vec{x}')}{dx} \right]_{x=x_i} \quad (25)$$

The right-hand part of formula (24) coincides by its form with the suggested in ref. [2-4] empirical expression for channeled fraction describing the dechanneling on defects. In those papers and in the other works (see, e.g., review [5] and references in it) the calculations of quantities σ_i named as "the dechanneling cross-sections of the defect i " for different concrete kinds of defects were given. As can be seen, the formula (25) is the rigorous general expression for dechanneling cross-sections σ_i . Note the essential dependence of σ_i on the distribution function $F(x)$ ("flux-peaking effect" for dechanneling on rough defects).

From the physical point of view it is reasonable to join all lengths $R_{ch}^i(z)$ and to regard them as a unit "defect dechanneling length" R_{ch}^d . Both the defect dechanneling length R_{ch}^d and the total dechanneling length R_{ch}^* are combined from R_{ch}^i and R_{ch} , just as we expected, according to the rule for calculation of total dechanneling length in the case, when several statistically independent factors α causing the dechanneling are doing simultaneously (see ref. [1])

$$(R_{ch}^*)^{-1} = \sum_{\alpha} (R_{ch}^{\alpha})^{-1} \quad (26)$$

Let us return now to expression (17) for channeled

fraction. Besides the exponential term there is in it a principally new second term, which is caused by the trapping of chaotically moving particles in the channeling regime. At this the quantity $R_r^{-1}(z)$ defined by (19) have the meaning of the intensities per unit path length of the processes of the capture of initially non-channeled particles in channeling regime. Therefore $R_r(z)$ is the rechanneling length.

Thus the main property of channeling with rechanneling lies in the existence, besides the dechanneling length R_{ch}^* , of new characteristic length defined above. Taking into account that chaotically moving particles can stop within comparatively short path lengths of order of projective range R_p , we may say that in the general case the dechanneling of charged particles would be described by three characteristic lengths: R_{ch}^* , R_r and R_p .

Since joined distribution function $F_r(z, x)$ is the sum of two functions with different initial conditions, we can split of the characteristic length R_r on dependent and not dependent parts from initial conditions:

$$[R_r^{p,s}(z)]^{-1} = \int_V dx \int_V dx' \frac{\vec{F}(x) \vec{F}(x')}{\|F\|^2} * \left\{ \sum_i \int_V dx'' \Phi_r^{p,s}(x'', z) \cdot w_i(z, \vec{x}'' \rightarrow \vec{x}') \right\} \quad (27)$$

This splitting may be necessary because distribution by x may be essentially different for channeling and non-channeling regimes.

In the general case, when $R_r^p(z)$ and $R_r^s(z)$ differ significantly, the expression (17) for dechanneling fraction has to be switched by the formula

$$P_c(z) = \int_V dx F_c(z, \vec{x}) = q \exp\left[-\frac{z}{R_{ch}^*}\right] + \int_0^z d\zeta \exp\left[-\frac{z-\zeta}{R_{ch}^*}\right] \left\{ \frac{P_r^p(\zeta)}{R_r^p(\zeta)} + \frac{P_r^s(\zeta)}{R_r^s(\zeta)} \right\} \quad (28)$$

In conclusion, let us discuss some properties of R_r . In the general case they depend on z , and this dependence is defined by the dependence on z of the function $\Phi_r(x, z)$. But since these functions are the solutions of the diffusion type equations, the dependence of R_r on z will be rather weak ($\sim z^{1/2}$ or $z^{3/2}$). And, at last, in the case of channeling of ions with not too high energies, when the projective range R_p is much smaller than dechanneling length R_{ch} and the crystal thickness, the length R_r are defined effectively by the distributions $\Phi_r(x, z \approx R_p)$ and, therefore, in this case they are constants.

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