THE RELATION BETWEEN DISCRETENESS AND THERMAL VIBRATIONS IN AXIAL CHANNELING

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The scattering cross section at atomic rows along crystallographic directions is an important characteristic in describing particle motion through single crystals under axial channeling conditions [1]. The effective-potential model [1] describes the elastic scattering involving conservation of the energy of the motion transverse to the axis of row (the transverse energy, for brevity). The main factors causing transverse-energy nonconservation are as follows: the discreteness in the atomic row [1-3] and the thermal motion of the atom [1,4], which are usually considered separately.

In this note, we discuss the relationship between these factors from numerical simulation results obtained by Monte Carlo methods for the scattering of fast protons ($Z_1 = 1$) of energy E = 500 keV by the principal atomic rows <100>, <110>, <111> in a germanium crystal ($Z_2 = 32$), which has the diamond structure. To establish the role of the row basis in the case of the angle <111> direction, we consider a hypothetical <111>* row with the same average interatomic distance d but without the basis.

See [5] for details of the calculation program and the scattering parameters of a <100> row in gold. We simulated the incidence of protons on a row from ∞ at an angle to the axis of the row θ_0, whose value was varied widely, while the crystal temperature T was varied from zero to the melting point. The resulting scattered-proton angular distributions were used to determine the angular quantity

$$\left\langle \frac{\delta\theta_n^2}{\delta z} \right\rangle = \frac{\langle\theta^2\rangle - \langle\theta_0^2\rangle}{\langle s\rangle},$$

which is proportional to the rate of increase with depth z in the mean transverse energy of the channel particles due to repeated scattering at the rows. Here s is the particle path in interaction with a row in an effective region of radius r_0,

$$r_0 = (\pi N d)^{-1/2},$$

where N is the density of atoms in the crystal and θ is the angle between the velocity vector and the row axis after collision. The angle brackets denote averaging over an ensemble of particles with a uniform distribution of the central collision parameters in the range $(0, r_0)$, which corresponds to averaging

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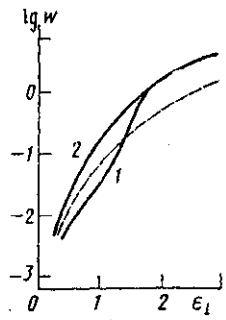

Fig. 1

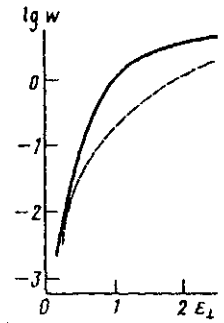

Fig. 2

Fig. 1. Dependence of the dimensionless characteristic w of the multiple proton scattering at E = 500 keV by atomic rows in germanium on the dimensionless transverse energy $\varepsilon_\perp$ for T = 48 K. The dashed line is the theoretical relationship of (2); simulation results: curve 1 for <111> direction, 2 for <110> and <100> directions and for a hypothetical <111>* row.

Fig. 2. Dependence of the dimensionless characteristic w of the multiple proton scattering at E = 500 keV by atomic rows in germanium on the dimensionless transverse energy $\varepsilon_\perp$ for T = 293 K; the dashed line is the theoretical relationship of (2), while the solid line is the simulation result for <110>, <100>, <111>, and <111>* rows in germanium.

over a statistically equilibrium particle distribution in axial channeling [1,5].

The dimensionless quantity

$$w = (\pi N b^2)^{-1} \left\langle \frac{\delta\theta_n^2}{\varepsilon z} \right\rangle, \quad b = \frac{Z_1 Z_2 e^2}{E} \tag{1}$$

is shown as a function of the dimensionless transverse energy $\varepsilon_\perp = 2\theta^2/\psi_1$, where ψ_1 is the Lindhard angle, for the cases of low temperatures (Fig. 1, T = 48 K) and room temperature (Fig. 2, T = 293 K). We also showed calculations on $\delta\theta^2/\delta z$ (or w_L) in the Lindhard model [1,6]:

$$\left(\frac{\delta\theta_n^2}{\delta z}\right)_L = \pi N b^2 w_L, \quad w_L = \frac{u_\perp^2}{C^2 a^2}\left(\exp(\varepsilon_\perp) + \frac{2}{3}\right)(1 - \exp(-\varepsilon_\perp))^3, \tag{2}$$

where $C^2 \approx 3$, a is the screening constant in the Thomas-Fermi model, and $u_\perp$ is the mean-square thermal displacement of the atoms in the transverse plane.

The results indicate that $w(\varepsilon_\perp, u_\perp)$ is a universal relationship for these rows in germanium, apart from a row with <111> basis at T = 48 K. In the latter case, the role of the row structure has an appreciable effect at sufficiently small transverse energies. Quantitative evaluation of the relation between the thermal and discrete factors can be based on the dimensionless parameter $\mu = u_\perp/r_D$, where r_D is the critical distance for using the effective-potential model [1,2]. In the case of the Lindhard form of potential, the solution to the equation for r_D [2] can be put approximately as

$$r_D \simeq 0{,}2568\,x(1+x/2);\ 0<x<2,\quad x=\frac{d}{a}\psi_1\sqrt{k}, \tag{3}$$

where k = 1 for chains without a basis and k = 7/2 for <111> chains with the diamond structure. Calculation from (3) showed that $\mu = 0.81$ for an <111> row at T = 48 K; $\mu > 1.8$ in the upper cases. This shows that the condition $\mu < 1$ is a necessary but sufficient condition for the discrete factor to predominate over the thermal one at low transverse energies. For $\mu > 1$, the thermal motion conceals the discreteness, and the relationships of (1) are universal for various crystallographic directions.

This conclusion is confirmed by the simulation results for quantities of the type of (1) for proton scattering by the principal atomic rows in FCC gold crystals over a wide temperature range, as well as the behavior of the energy losses on interaction with atomic electrons and the back-scattering yield in channeling in these crystals [7].

Comparison of the numerical calculations (1) and the analytic ones (2) shows that (2) is applicable in a restricted range of small transverse energies $\varepsilon_\perp < \varepsilon^*_\perp$, $\varepsilon^*_\perp \sim \ln(1+C^2a^2/u^2_\perp)$. This conclusion still applies when one incorporates the subsequent terms in $(u_\perp/(Ca))^2$ in (2), which requires more careful analytical calculations to describe the functions of (1) over a wide transverse-energy range.

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