Energy dependence of the electron angular distributions during planar channeling

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The angular distributions of the relativistic electrons transmitted through a silicon crystal have been measured under {110}-plane channeling conditions. The results reveal an alternation of "two-humped" and "three-humped" distributions as the electron energy is raised from 0.85 to 5.4 MeV. A theory is derived for the effect. The effect is shown to result from a shift of the energy bands and an unusual attendant change in the structure of the wave functions of the states above the potential barrier.

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1. Low-lying states above the potential barrier play a special role in the channeling of fast electrons, giving rise to a group of electrons which undergo a weakened inelastic interaction with the crystal atoms.[1] Under these conditions the relativistic mass of the channeled particles becomes a parameter which can be varied to control the position of the energy bands above the barrier and thus to make important changes in the nature of the channeling.

In the present study we have observed a clearly defined dependence of the angular distribution of electrons transmitted through a crystal under planar-channeling conditions on the energy of the incident beam. There is an alternation of very different "two-humped" and "three-humped" structures. The changes result directly from a shift of the energy bands in the effective potential of the crystallographic planes with increasing relativistic mass of the incident particles and from a corresponding, extremely unusual change in the properties of the wave functions of the low-lying states above the barrier.

2. The experiments were carried out at intermediate energies with a high-voltage electron diffraction camera using a Van de Graaf accelerator and a microtron. The total electron energy $E = mc^2\gamma$ lay in the range 0.85–5.4 MeV. The angular divergence of the incident beams, 0.03–0.1°, was smaller than the corresponding critical angles for {110}-plane channeling in silicon. Figure 1 shows some electron angular distributions obtained through photometric measurements of electron diffraction patterns recorded in experiments in which the beam axes were parallel to the system of {110} planes of a silicon crystal $L = 5$ μm thick.

At $E = 850$ keV the diffraction pattern has two spots of elevated intensity, which correspond to two peaks on the electron angular distribution, in symmetric positions at $\phi = \pm 0.25°$. At $E = 1.3$ MeV, the two peaks move closer together ($\phi = \pm 0.13°$), and

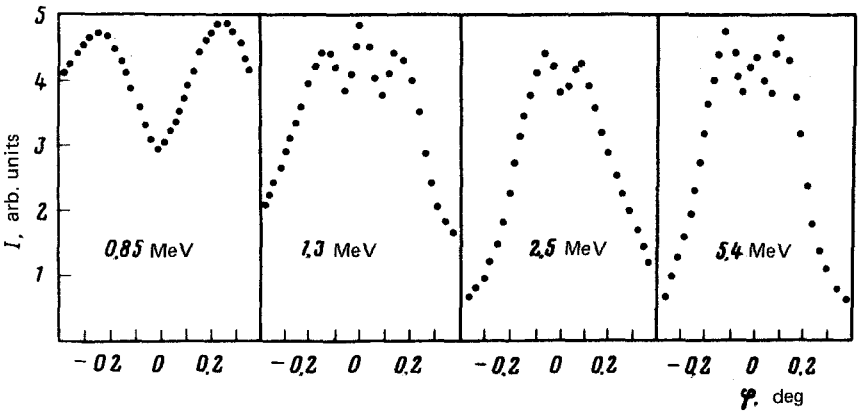

FIG. 1. Experimental angular distributions of electrons in the plane which is orthogonal to the plane {110} planes of silicon and which passes through the axis of the incident beam.

a third peak appears along the direction of the crystallographic plane ($\phi = 0$). At $E = 2$ MeV, the angular distribution returns to its two-humped shape, with peaks at $\phi = \pm 0.1°$. At the higher energy of 2.5 MeV, the distribution still has two peaks, which are now shifted to $\phi = \pm 0.07°$. At $E = 5.4$ MeV, there are three peaks, as at $E = 1.3$ MeV: a central peak along the direction of the plane and two side peaks at $\phi = \pm 0.1°$.

3. An important consideration for a qualitative analysis of the effect is that the thickness of the crystal used in these experiments is more than an order of magnitude greater than the mean free path of the incident electrons in an amorphous medium of the corresponding composition and density. Since, in this energy range, this mean free path is actually the decay length for the off-diagonal elements of the particle density matrix in the Bloch-function representation,[2,3] no coherent effects caused by an interference of different Bloch states should occur where the electrons leave the crystal. Furthermore, the fact that the electrons in states below the barrier are strongly scattered by crystal atoms over this crystal thickness[1] directly implies that the "anomalous" part of the angular distribution, which has the fine structure with two or three peaks, is determined by electrons which are in a low-lying band above the barrier and which interact relatively weakly with the crystal atoms.

On the basis of simple physical considerations we may assume that all values of the quasimomentum q ($|q| \leqslant \pi/d$, where d is the distance between planes) in the corresponding band are populated nearly uniformly when the electrons leave the crystal, so that the problem reduces to one of analyzing the properties of the wave functions of low-lying states above the barrier, a_{nq}, in the momentum representation. The square moduli of these wave functions should describe the structure observed in the electron angular distribution.

4. For potentials with a center of inversion, the behavior of $|a_{nq}|^2$ at small q is determined primarily by the symmetry properties of the corresponding Bloch functions $\Psi_{nq}(x)$ in the coordinate representation. If, for example, the function $\psi_{nq}(x)$ is of odd parity with respect to x at $q = 0$ in a low-lying band above the barrier, then the corresponding $a_{nq}|_{q=0}$ is zero, and the electron angular distribution at the exit

from the crystal has a minimum along the direction of the $\{110\}$ plane. Since the typical momentum of a particle in such a state is approximately $\sqrt{2EV_0}/c$, the maxima of $|a_{nq}|^2$ occur at angles

$$\phi \approx \pm \frac{1}{2}\left(\frac{2EV_0}{E^2 - E_0^2}\right)^{1/2}, \tag{1}$$

where V_0 is the height of the potential barrier, and $E_0 = mc^2$ is the rest energy of the electron.

The parity of the corresponding Bloch function at $q = 0$, on the other hand, directly implies $|a_{nq}|^2_{\phi=0} \neq 0$. Since the particles "linger" in the regions above the potential barriers, we then easily see that the region near $\phi = 0$ should be emphasized in the angular distribution along with the angles in (1). Whether the angular distribution of $|a_{nq}|^2$ has a maximum at $\phi = 0$ in this case, and if so what the size of this maximum is, depends on the position of the above-barrier band with respect to the crest of the potential barrier.

5. The most significant feature in this entire picture is that for motion of electrons with a small relativistic mass in the potential of the silicon $\{110\}$ planes the second energy band at $q = 0$ has an even-parity wave function.

As the mass of the particle increases, this band is gradually "pulled" into the potential well, and it ultimately converts into a below-barrier band. The wave function of the Bloch state with $q = 0$ in the second below-barrier band, however, is evidently of odd parity. At a certain value of the mass in this band there should accordingly be a change in the parity of the wave function with $q = 0$.

A detailed analysis shows that this change in parity occurs above the barrier, at a relativistic mass at which the energy of the top of the second band completely suppresses reflection from the potential well, which forms a separate unit of the effective periodic potential. The width of the energy gap between the second and third bands vanishes here, and a degeneracy arises for the given value of the transverse energy.

6. In summary, we find the following qualitative picture of the energy dependence of the electron angular distribution for $\{110\}$-plane channeling in silicon in this energy range.

At low energies E, because of the rather high position of the second band above the potential barrier (the first band is entirely a below-barrier band at all values of E), the electron angular distribution is two-humped with a minimum at $\phi = 0$. As the energy is raised, this minimum converts into a maximum because of the lowering of the second band; the relative height of this maximum in the three-humped pattern increases until the parity of the wave function with $q = 0$ changes in the second band. Starting at this value of E, and continuing until the second band is completely "pulled" below the barrier, the electron angular distribution is again a symmetric two-humped distribution. At this point a third band, having a wave function of even parity at $q = 0$, comes into play, and the angular distribution becomes a symmetric three-humped distribution with a clearly defined central maximum.

7. Corresponding calculations have been carried out in the model of planar channeling with a Kronig-Penney potential.[4] The potential well had the usual depth,

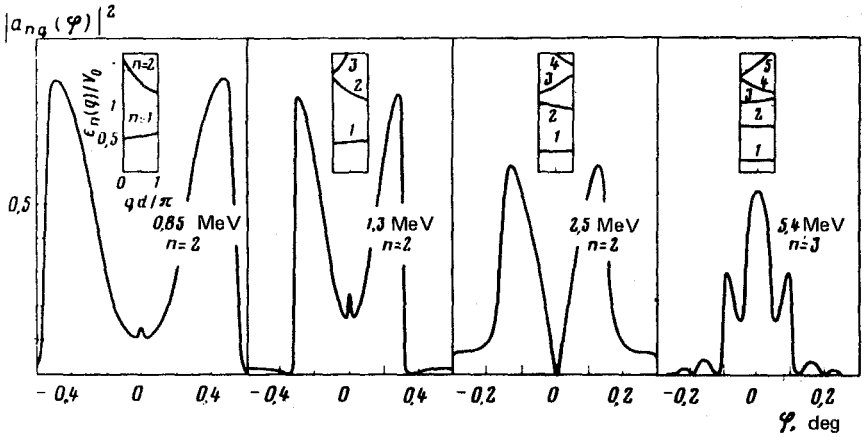

FIG. 2. Band structure of the transverse-motion energy levels and angular distributions for electrons in low-lying bands above the barrier according to the Kronig-Penney model, with the parameters given in the text proper.

$V_0 = 24$ eV, while the width of the well, $a = d/3 = 0.64$ Å, was chosen in such a way that the "bottom" of the second energy band would touch the crest of the potential barrier at an electron energy of about 2 MeV, as actually occurs in practice.

The energy parameters of the motion of the low-lying bands above the barrier in this model are as follows: The change in the parity of the Bloch function with $q = 0$ in the second band occurs at $E = E^{(2)}_{\text{even}} = 1.47$ MeV; the bottom and top of the second band touch the crest of the barrier at $E^{(2)}_{\text{touch}} = 1.96$ MeV; $E^{(2)}_{\text{gap}} = 2.68$ MeV; and the corresponding energy for the third band is $E^{(3)}_{\text{touch}} = 7.84$ MeV.

The calculated angular distributions (Fig. 2) are in qualitative agreement with the experimental data.

Interestingly, in the Kronig-Penney model we have

$$E^{(2)}_{\text{even}} = E^{(2)}_{\text{touch}}\left[1 - \left(\frac{a}{d-a}\right)^2\right]. \tag{2}$$

In reality, on the other hand, since the potential of the silicon $\{110\}$ planes is approximately the Pöschl-Teller potential,[2] for which the reflection coefficient at an individual potential well becomes zero at $E \cong E^{(2)}_{\text{touch}}$, we have

$$E^{(2)}_{\text{even}} \cong E^{(2)}_{\text{touch}}, \tag{3}$$

and the lower position of the above-barrier bands causes the central peak in the three-humped experimental angular distribution at $E < E^{(2)}_{\text{even}}$ to be more pronounced than in this model-based calculation.

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