Energy limits of Bragg diffraction of charged particles in a single crystal

S. L. Dudarev and M. I. Ryazanov
Engineering Physics Institute, Moscow

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It is shown that diffraction of fast charged particles in a single crystal vanishes with increasing particle energy. The temperature dependence of the effect is found.

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1. Bragg diffraction of charged particles consists of their reflection from a system of crystallographic planes by small angles. If we are not interested in channeling,[1,2] then the angle of reflection is greater than the Lindhard critical angle θ_L. The angle of reflection due to diffraction is related to the reciprocal lattice vector g by the relation

$$\theta \approx 2\sin(\theta/2) = (\hbar g/p).$$

The condition $\theta/2 > \theta_L = \sqrt{2EV_0}/pc$ means that diffraction occurs only for the values

$$g > g_{min} = \frac{1}{\hbar c}\sqrt{8EV_0}\,, \tag{1}$$

where V_0 is the effective potential barrier of the channel. Thus the region of Bragg diffraction has a lower limit.

2. On the other hand, the existence of incoherent quasielastic scattering by thermally induced fluctuations of the potential limits the region of existence of Bragg scattering from above. The necessity of exact orientation of the velocity of the particles relative to the crystallographic planes for Bragg diffraction leads to the fact that under normal conditions (thermal displacement u_a of the order of the screening radius) even single incoherent scattering removes the particle from the Bragg direction. The characteristic diffraction reflection length is the "pendulous" length[3]

$$l_M(\mathbf{g}) = \frac{\hbar v}{n\,|U(\mathbf{g})|}\exp\left(\frac{1}{2} < (\mathbf{g}\,\mathbf{u})^2 >\right),$$

where n is the number of atoms per unit volume, and $U(\mathbf{q})$ is the Fourier transform of the atomic potential. Diffraction vanishes if the probability of incoherent scattering at this length is of the order of unity. Thermally induced fluctuations in the potential of a separate atom

$$\delta U_a = U(\mathbf{r} - \mathbf{R}_a - \mathbf{u}_a) - < U(\mathbf{r} - \mathbf{R}_a - \mathbf{u}_a) >$$

in the approximation of uncorrelated thermal displacements gives the following scattering cross section[4]

$$\sigma = \int d\sigma_0 (1 - \exp(- <(\mathbf{q}\,\mathbf{u})^2 >)), \tag{2}$$

where σ is the cross section for scattering by an isolated atom. For this reason, the following inequality is the condition for vanishing of diffraction:

$$l_M(g)\, n\sigma \gtrsim 1\,. \tag{3}$$

We emphasize that σ does not depend on g, while $l_M(g)$ increases with increasing g. For this reason, inequality (3) actually sets a limit for the region of existence of Bragg scattering for large g. The upper limit $g_{\max}$ of the region of reciprocal lattice vectors g, for which diffraction exists, is the root of the equation

$$\sigma = \frac{1}{\hbar v}\,|U(\mathbf{g})|\exp\left(-\frac{1}{2} <(\mathbf{g}\mathbf{u})^2 >\right). \tag{4}$$

3. It is significant that the cross section and, therefore, $g_{\max}$ in (4) is a function of the velocity, rather than the energy of the particle, i.e., it is nearly independent of energy for $v \sim c$. At the same time, the lower boundary of the region of diffraction is $g_{\min} \sim \sqrt{E}$. As the particle energy is increased, the region of diffraction therefore narrows and vanishes at

$$E > E_{crit} \cong \frac{c^2\hbar^2}{4V_0 <u^2>} \ln\left(\frac{|U(g_{min})|}{\hbar v\sigma}\right). \tag{5}$$

For particles with energies exceeding $E_{\rm crit}$, incoherent scattering by thermal fluctuations of the potential with cross section (2), similar to multiple scattering in an amorphous medium, dominates everywhere outside the region of channeling. As follows from the analysis performed in Ref. 5, the quantity V_0 decreases with the transition to systems with crystallographic planes with high Miller indices, and Bragg diffraction for $g < g_{\max}$ exists up to higher particle energies. On the other hand, such loosely packed planes[5] correspond to large values of $g(hkl)$ and inequality (3) is satisfied even for reflection by the first vector $g_1(hkl)$. This fact accounts for the absence of coherent phenomena with motion of particles along loosely packed planes. As follows from (4), for temperatures above the Debye temperature, the critical energy decreases as T^{-1}. At $T = 300$ K, for (110) planes in silicon $E_{\rm crit} \cong 5$ MeV.

4. Thus, for high-energy electrons, $E > E_{crit}$, a single crystal is either in the channeling regime at $\theta < \theta_L$ or incoherent scattering occurs in it at $\theta > \theta_L$, while Bragg scattering is found to be missing. This effect greatly influences the reflection of relativistic electrons from a single-crystal surface, discussed in Ref. 6. In particular, reflection at $E > E_{crit}$ outside the region of channeling occurs in a manner similar to the reflection from an amorphous medium. In the case of pendulous radiation of electrons, the indicated vanishing of diffraction will strongly suppress the radiation of high-energy electrons examined in Ref. 7, if the Bragg-reflection limits are ignored.

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