Anomalous channeling and quasicharacteristic radiation of nonrelativistic electrons in ionic crystals

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Orientational motion of low-energy electrons is shown to occur in Li^+ (111) planes of light ionic crystals like LiH and LiD at anomalously great depths, so that effective quasicharacteristic radiation may be generated. This is due to, firstly, the presence of two important features, namely, a low electron density in the channeling regions and a high charged particle binding energy; secondly, this is due to an anomalous inversion of the structure of the potential, transforming a potential well in an H^- plane into a barrier.

It is regarded as obvious that channeling and quasicharacteristic radiation of nonrelativistic electrons are impossible in principle (see the reviews in Refs. 1 and 2). The reasons are the small depth and width of a well for such particles. Even when the potential does admit the presence of at least one bound-motion level, the very strong deceleration and scattering of particles moving in a region with a high atomic density make the length of regular motion (effective dechanneling length) extremely short, $\Delta z_d \ll 1\ \mu$m, which excludes the possibility of utilizing the effect.

Only if $E_0 \lesssim 1$ MeV is it possible to channel electrons in crystals of moderate average atomic weight and in the range $E_1 \lesssim 2$–3 MeV there is already a pair of levels, so that we can consider the problem of short-wavelength radiation. Even if weakly relativistic electrons do penetrate to a much greater depth than nonrelativistic electrons, they still move in regions with a higher electron density, which has a very strong effect on their propagation (for example, for $E = 4$ MeV the dechanneling length is $\Delta z_d \approx 0.03\ \mu$m for an Si crystal[3]) and, consequently, it also affects the quality of quasicharacteristic radiation (the intensity of the radiation is low and the spectrum is very broad). These shortcomings demonstrate the low efficiency of weakly relativistic electrons as sources of quasicharacteristic radiation and particularly the unsuitability of particles of energy $E \lesssim 1$ MeV for this purpose.

What are the alternatives? We can use channeling of positive particles, such as positrons. They travel between planes in regions with a lower electron density. However, beams with high positron densities cannot yet be generated.

We shall propose a different approach and show that for orientational motion of low-energy electrons in light ionic crystals like LiH and LiD we can expect efficient generation of quasicharacteristic short-wavelength radiation. However, in contrast to Ref. 4, where electrically neutral (100) and (110) planes are selected, we shall concentrate our attention on charged (111) planes in which—as shown below—the dechanneling length is longest, reaching tens of microns. Moreover, the average electron potential of LiH in a (111) plane is characterized by an anomalous inversion effect representing transformation of a potential well in an H^- plane into a barrier. These results are due to overcompensation of the smallest (among all other possible) charge in an H plane by the "excess" electron from Li acquired in the course of ionic bond formation, which reduces very greatly the depth of the well (from 10 eV for hypothetical atomic hydrogen planes to 1.8 eV for H^- planes in an LiH crystal); the well vanishes at the temperature corresponding to flattening of the potential.

We shall calculate this potential for one period allowing for the influence of all the planes in the crystal. We choose the coordinate system so that the yz plane coincides with the Li^+ plane. In constructing the potential we shall allow for the following: in the case of an LiH crystal with an almost complete exchange of electrons between atoms (because the degree of ionicity in this crystal is within the range 0.8–1—see Ref. 5) the electron shell of Li^+ resembles that of He, but with the nuclear charge the same as for Li. Similarly, in the case of H planes the shell corresponds to He, but the nuclear charge is that of H. Consequently, the planar potential is established as a result of influence of two types of distorted rare-gas neutral atoms (Li→He, H→He) and by the combined effect of planes carrying charges of alternating signs. Bearing these points in mind and then calculating the one-particle potentials of the interaction of an electron with distorted helium atoms using the Gauss theorem, we obtain the following potential after the usual procedures of averaging over the planes:

$$V(x) = -2\pi e^2 g\left\{\exp\left(-\frac{2Z_1^*}{a_0}|x|\right)\left(|x| + \frac{3a_0}{2Z_1^*}\right) - |x| + F^{(+)}(x) + F^{(-)}(x)\right\},$$

$$F^{(\pm)}(x) = \left[\left|x \pm \frac{a}{2\sqrt{3}}\right| + \frac{3a_0}{2Z_2^*}\right]\exp\left[-\frac{2Z_2^*}{a_0}\left|x \pm \frac{a}{2\sqrt{3}}\right|\right],$$

which is specified for one period $|x| \leqslant a/2\sqrt{3} \approx 1.18$ Å. Here, $g = 4/a^2\sqrt{5}$ is the density of atoms in the (111) planes; a is the lattice constant of the crystal; a_0 is the Bohr radius; $Z_{1,2}^* = Z_{1,2} - \beta$ are the effective nuclear changes of the Li^+ and H^- ions (after allowance for the screening parameter $\beta = 5/16$—see Ref. 6). We can easily show that this potential satisfies the requirement

$$\partial V(x+0)/\partial x - \partial V(x-0)/\partial x = 4\pi e\sigma(x)$$

at any point {including at "frozen" Li^+ and H^- planes when the surface charge density is described by the relationship $\sigma(x) = ge\{Z_1\delta(x) + Z_2\delta(|x| - a/2\sqrt{3}\}$. The structure of such a "frozen" potential is represented by trace 1 in Fig. 2 after subtraction of the constant component. The next (customary in such cases) step is the averaging over the phonon vibrations, i.e.,

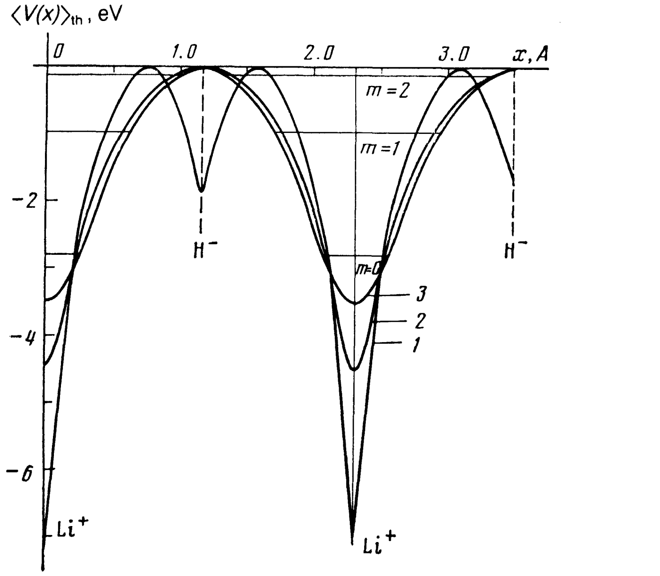

FIG. 1. Structure of electron interaction potentials in (111) planes of an LiH crystal in the "frozen" case when the mean-square displacements of the ions u_1 and u_2 are zero (curve 1) and in the case of phonon flattening at $T = 0$ K and $T = 300$ K (curves 2 and 3, respectively). In the last case the levels of the channeled electrons are shown for $E = 20$ MeV.

$$\langle V(x)\rangle_{th} = \int_{-\infty}^{\infty} V(x-y) f(y)\, dy,$$

where $f(y) = (2\pi u^2)^{-1/2} \exp(-y^2/2u^2)$ is the function of fluctuating deviations of atoms from their equilibrium positions and u is the mean-square amplitude of the ion thermal vibrations. It is necessary to carry out tanh averaging separately for the Li^+ and H^- planes, in which the displacements of the ions are $u_1 = u(Li^+)$ and $u_2 = u(H^-)$, respectively. A table of the values of u_1 and u_2 obtained for various temperatures is given in Ref. 5. The dependences $\langle V(x)\rangle_{th}$, such as those at two temperatures $T = 0$ and $T = 300$ K are also shown in Fig. 1 (curves 2 and 3, respectively). The values of u_1 and u_2 are 0.156 and 0.252 Å in the former case and 0.215 and 0.271 Å in the latter case.[5] From this figure follows the property of the potential noted above, namely, the appearance of barriers to electrons in the H^- planes in place of the potential wells, beginning literally at $T = 0$ K. The potentials of an LiH crystal in the electrically neutral (100) and (110) planes[4] naturally do not exhibit this feature.

In analyzing the actual spectrum we shall select the potential $\langle V(x)\rangle_{th}$ at $T = 300$ K and approximate it by a function of the type $U(x) = -U_0/\cosh^2(x/b)$ with the parameters $U_0 \approx 3.5$ eV and $b \approx 0.5$ Å. Solving the Schrödinger equation with the relativistic mass $\mu\gamma$, we obtain a spectrum of energy levels of transverse motion[7]

$$E_{m\perp} = -\frac{\hbar^2}{2\mu\gamma b^2}(s-m)^2, \quad m = 0, 1, \ldots, \lfloor s \rfloor;$$

$$s = (2\mu\gamma U_0 b^2/\hbar^2 + 1/4)^{1/2} - 1/2.$$

The wave functions for the two lowest levels of interest to us are of the form [$B(s, s)$ is the beta function]

$$\psi_0(x) = \frac{1}{2^s}\left[\frac{2}{bB(s,s)}\right]^{1/2}\left(\mathrm{ch}\frac{x}{b}\right)^{-s},$$

$$\psi_1(x) = \frac{1}{2^{s-1}}\left[\frac{s-1}{bB(s,s)}\right]^{1/2}\mathrm{sh}\frac{x}{b}\left(\mathrm{ch}\frac{x}{b}\right)^{-s}.$$

Numerical estimates similar to those given above show that at nonrelativistic energies $E \lesssim 0.5$ MeV the dechanneling length for the motion in the first quantum level attains an acceptable value $\Delta z_d \approx 0.5$ μm. High-quality quasicharacteristic radiation can be generated employing electron beams of moderate energy $E \approx 20$–30 MeV. In fact, at this energy the lower levels are sufficiently deep (Fig. 1), i.e., the main level-broadening mechanism remains the dechanneling effect. The partial dechanneling lengths for these levels can be estimated from the results obtained using the quantum theory of electron scattering in the course of their channeling,[8] i.e., Δz_{dm} is governed by $\hbar c/\Delta E_m$, where ΔE_m is the broadening due to the finite lifetime of electrons at the levels due to elastic scattering and it is described by

$$\Delta E_m \approx \frac{2g}{\pi\hbar c}\int_{-\infty}^{\infty} dy \left\{ \int_0^{\infty} dq\, [(v_q^2)_{mm} - (|v_q|_{mm})^2] \right\} f(y).$$

Here, q is the change in the momentum of a p electron in the longitudinal direction, $v_q(x-y)$ is the Fourier transform of the one-particle potential, the planar average of which yields $U(x)$, and the parentheses with indices mm denote the following weighted average: $(\ldots)_{mm} = \int dx |\psi_m(x)|^2(\ldots)$. Calculations yield $\Delta z_{d(0,1)} \approx 25$ μm, which is over an order of magnitude greater than the value obtained in the case of conventional channeling.

An important advantage is also that the energy $E \approx 20$ MeV is optimal for this potential from the point of view of achieving the maximum inversion [$\Gamma(x)$ is the gamma function]:

$$\Delta W_{10}(\theta_0) = W_1(\theta_0) - W_0(\theta_0) = \frac{b\sqrt{3}\,\Gamma(2s)}{2a\Gamma^4(s)}\left\{2(s-1)\left(\frac{pb\theta_0}{2\hbar}\right)^2 \times \left|\Gamma\left(\frac{s-1}{2} - i\frac{pb\theta_0}{2\hbar}\right)\right|^4 - \left|\Gamma\left(\frac{s}{2} - i\frac{pb\theta_0}{2\hbar}\right)\right|^4\right\}$$

for the optimal angle θ_0 of entry to the crystal. The dependence $\Delta W_{10}(\theta_0)$ on the parameter s, related directly to E is plotted in Fig. 2 and we can see that $\Delta W_{10}^{max}(\theta_0) \approx 0.18$.

A direct application of the usual formula for the probability of spontaneous emission (see, for example, Ref. 2) $A_{10} = 4e^2\omega_{10}^3 x_{10}^2 \gamma^2/3\hbar c^3$, carried out using the matrix element $x_{10} = ((s-1)/2)^{1/2} b (\Gamma(s-1/2)/\Gamma(s))^2$ and the

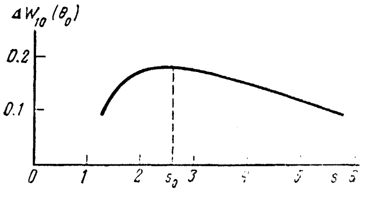

FIG. 2. Population inversion $\Delta W_{10}(\theta_0)$ between the two lowest energy levels calculated for the optimal angle θ_0 of entry into a crystal as a function of the parameter s.

functions ψ_0 and ψ_1, yields the following estimate for the number of photons of energy $\hbar\omega_{max} \approx 2\gamma^2\hbar\omega_{10} \approx 6$ keV, corresponding to a transition of frequency of $\omega_{10} = \hbar(2s-1)/2\mu b^2\gamma$ lying in the visible part of the spectrum, per incident electron with velocity v: $N_1 \approx A_{10}\langle\Delta z_d\rangle\Delta W_{10}/v \approx 2\cdot 10^{-5}$ photons/electron. This is at least an order of magnitude greater than in the case of the usual channeling in crystals.[3]

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