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Channeling radiation from relativistic electrons in LIF crystal: when a classical description is valid?

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Introduction

The channeling radiation (CR) from moderately relativistic particles in diatomic crystals has been studied first by in [1]. Recently, the LiF crystal was applied as a promising radiator for generation of parametric X-Radiation [2].
In the theory of channeling radiation, the crystals like LiF are interesting from the point of view of non-trivial planar and axial potentials, which form the specific energy level structure of transverse motion responsible for CR spectrum. In turn, the transverse energy levels scheme depends on the incident particle energy.
We investigated the quantum versus classical description of CR in LiF (and similar crystals) using a quantum approach as in [3] and classical approach as in [4], and analyzed the CR spectra which may combine simultaneously both quantum and classical features.

Continuous planar potential for (111) channeling in LiF

For calculation of planar channeling is used one-dimensional continuum potential $V(z)$ averaged along the longitudinal directions (x,y)

$$V(z) = \sum \frac{1}{S} \int_S V(\mathbf{r}) dx dy,$$

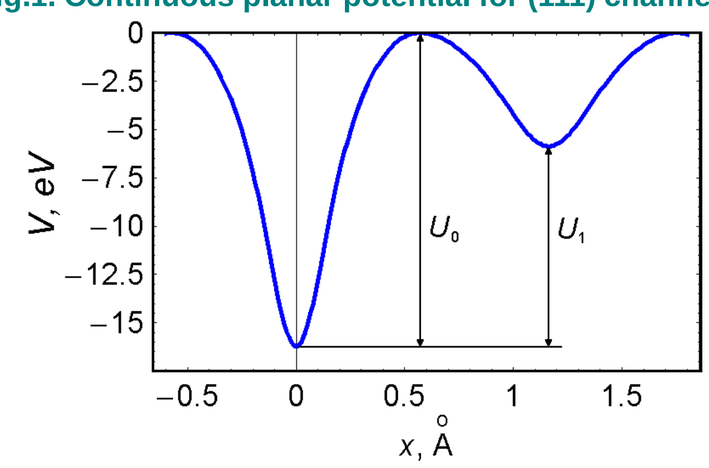
where $V(\mathbf{r})$ - potential due to a single atom of the plane and the integration is over all planes, S - area fall on the single atom. The summation is carried out over all planes which are perpendicular to Z direction.
For calculation of potential of an atom the electron scattering form factor was used [5] which is Fourier transform of potential $V(\mathbf{r})$:

$$f_e(s) = \frac{2m_0}{\hbar^2} \int_0^\infty V(\mathbf{r}) r^2 \frac{\sin 4\pi s r}{4\pi s r} dr,$$

where m_0 is electron mass, $s=\sin\theta_r/\lambda$, θ_r - scattering angle of an electron with wavelength λ. The analytic approximation of f_e was obtained by fitting to six Gaussians.

$$f_e(s) = \sum_{i=1}^{6} a_i \exp(-b_i s^2).$$

Fig.1. Continuous planar potential for (111) channeling in LiF



Classical description of planar CR

Equation of motion of a relativistic electron in the potential (Fig. 1), for transverse direction

$$\gamma m \ddot{x} = F = -\frac{\partial U(x)}{\partial x}, \gamma = \frac{1}{\sqrt{1-\upsilon_{||}^2/c^2}}.$$

- Assumptions $\upsilon_\perp \equiv \dot{x} << \upsilon_{||}; \upsilon_\perp/c << 1/\gamma$, $\upsilon_{||}$ is average speed of electron
- Initial conditions: incident point into a crystal $x(0) \equiv x_0$, transverse momentum $p_\perp(0) \equiv p_{||}\theta_0$
  θ_0 is incidence angle of an electron on channeling plane
- Transverse energy

$$\varepsilon_\perp = U(x) + \frac{\mathbf{p}_\perp^2}{2\gamma m} = U(x_0) + \frac{\mathbf{p}_{||}{}^2\theta_0^2}{2\gamma m}.$$

Trajectories and velocities of particles are obtained by numerical integration of equation of motion, without taking into account of dechanneling. The Fourier components of velocity are necessary for CR spectra calculation:

$$\frac{dW}{d\omega dz} = \frac{e^2\omega}{c^4T^2} \sum_{l=1}^{\infty} \Theta[1-\eta_l] \cdot \left[\eta_l^2 - \eta_l + \frac{1}{2}\right] \cdot |\dot{x}_{\tilde{\omega}}|^2;$$

$$\eta_l = \frac{T\omega}{2\pi\gamma^2 l}, \tilde{\omega} = \frac{2\pi l}{T}, \dot{x}_{\tilde{\omega}} = \int_{-T/2}^{T/2} \dot{x} e^{i\tilde{\omega}t} dt,$$

$\Theta[1-\eta_l]$ is the theta-function; T is oscillation period of electron in the planar channel

Quantum description of planar CR

Wave function φ_i was obtained from Schrodinger equation with relativistic mass $m^*=\gamma m_e$ and Bloch boundary conditions. Probability of spontaneous transition from a state i into a state f, according of quantum electrodynamics formula [6]

$$W_{if} = \frac{ce^2}{2\pi\hbar} \int \Phi \frac{\delta(\omega_{if}-\omega)}{k} d^3\mathbf{k} \qquad |\mathbf{k}| = \omega/c$$ – wave vector of a photon

It is possible to derive a simple expression for CR photon energy, if energy of transverse motion of electron is much smaller than total electron energy:

$$\hbar\Omega_{if} = E_i(k_j) - E_f(k_j), \omega_{if} = \Omega_{if} + ck\cos\theta, \Phi = \chi_{if}^2 \left[\cos^2\xi \left(\frac{\cos\theta - \beta_{||}}{1-\beta_{||}\cos\theta}\right)^2 + \sin^2\xi\right],$$

θ is angle between wave vector and Z axes, ξ - polar angle of wave vector in XY plane

The matrix elements: $\chi_{if} = \int e^{-ikx} \varphi_i^*(k_j, x) \varphi_f(k_j, x) dx$

Spectral distribution of CR:

$$\frac{dI}{d\omega} = \hbar\omega \frac{dW_{if}}{d\omega} = \sum_i \sum_{f\neq i} \frac{dI_{if}}{d\omega} = \alpha\hbar\omega \sum_i \sum_{f\neq i} \chi_{if} \left[1 - 2\frac{\omega}{\omega_m} + 2\left(\frac{\omega}{\omega_m}\right)^2\right] P_i,$$

α is fine-structure constant, P_i - initial populations of the i band, $\omega_m = \hbar\Omega_{if}/(1-\beta_{||})$

The matrix elements were determined numerically without of use of dipole approximation. CR spectrums calculated with and without of dipole approximation are shown in Fig. 3.

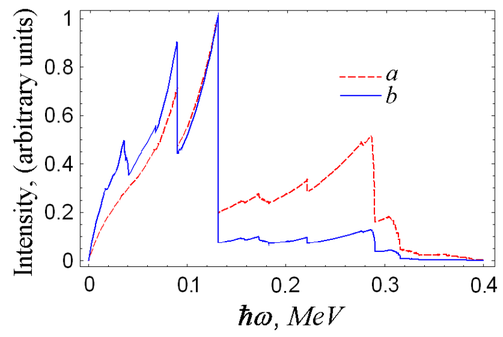


Fig. 3. CR spectra: *a* - dipole approximation, *b* - without of dipole approximation

CR spectra in (111) LiF: comparison of quantum and classical calculations

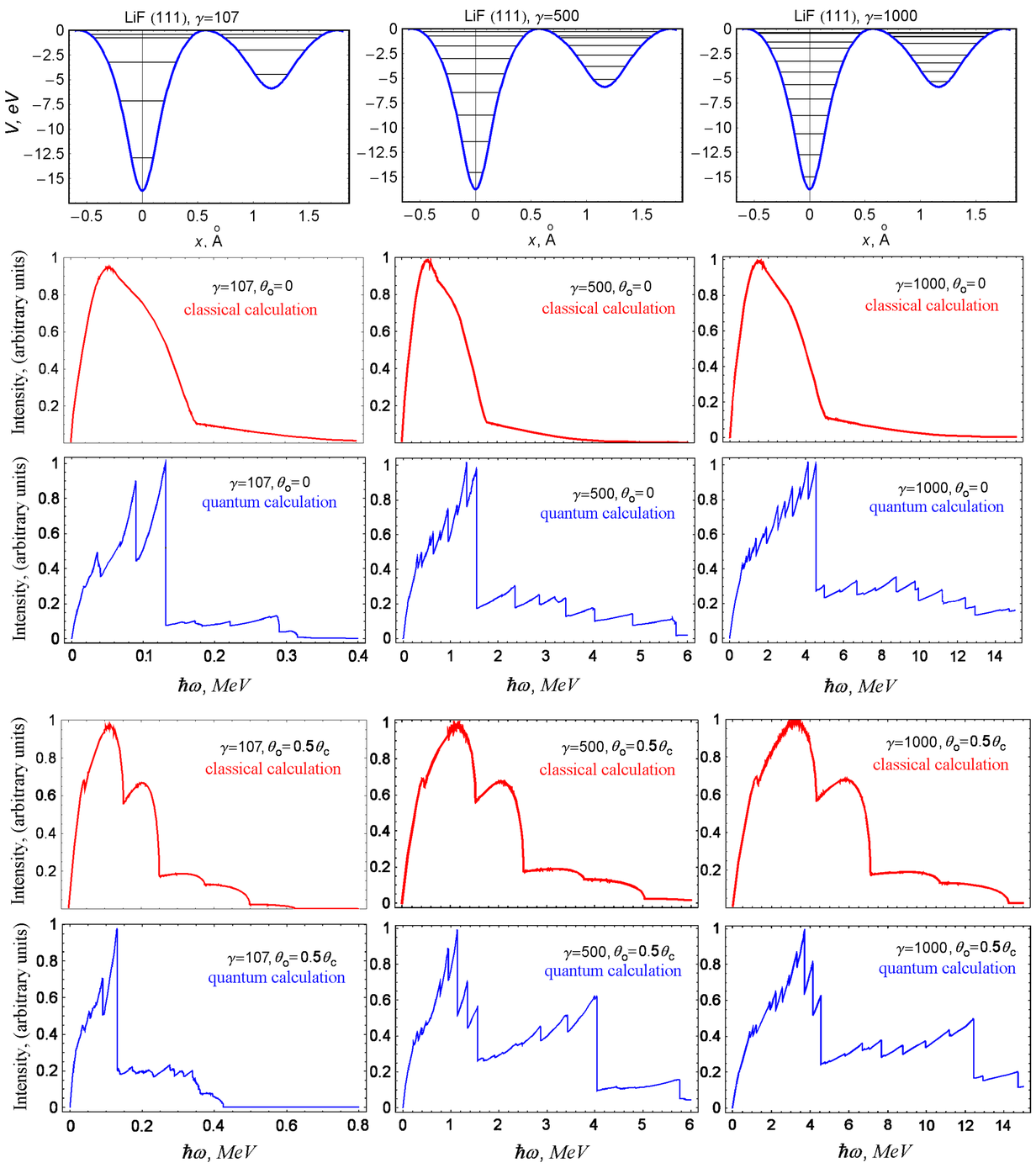


Fig. 4. Transverse energy levels and CR spectra calculated using classical (red), and quantum approach (dark blue) for different relativistic factors and incident angles

Conclusions

- Positions of main spectral maxima of CR well coincide in quantum and classical consideration, especially at incident angles greater than zero
- With increase of relativistic factor from 107 to 1000 the number of transverse energy levels increases from 5 and 4 up to 14 and 10 in small and deep potential wells correspondingly. Although relativistic factor becomes large enough, the problem of CR in LiF still remains quantum
- With increase of relativistic factor the CR spectra calculated in quantum approach became more complicated because of increase of transverse energy levels number.
- Calculated features of CR spectra in LiF crystal allow to use this crystal as perspective target for generating of hard X-rays (above 50 keV) and gamma-radiation (with photon energy up to 2 MeV).

References

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