INTERACTION OF RELATIVISTIC PARTICLES WITH CRYSTALS AND MATTER

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PECULIARITIES OF CHANNELING AND GENERATED RADIATION OF RELATIVISTIC ELECTRONS IN THE MAIN CHARGED AXES OF LITHIUM HYDRIDE CRYSTAL

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The paper deals with the calculation of electron interaction potentials with the main charged [110] axes in a lithium hydride crystal at T = 300, 600, and 900 K temperatures. For relativistic electrons with Lorentz factors $\gamma = 50, 75, 100$ the energy and corresponding wave functions of transverse levels of channeling motion are found numerically. The radiation spectra of channeling electrons with (and without) accounting an angular dispersion are calculated on the basis of these data.

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INTRODUCTION

In [1, 2] experimental investigations of a short wave radiation generated at the channeling of relativistic electrons with a longitudinal energy $\varepsilon_{\|} \approx 54$ MeV in main crystallographic planes (100), (110), and (111) of LiH and LiD crystals were carried out. These lightest ionic crystals with a NaCl-type structure have a number of unique characteristics [3]. For example, they have minimum electron density and are characterized by a very large dechanneling length. In [2] the attention was focused on the peculiarity of channeled radiation (CR) spectra in charged planes (111) of these crystals that deals with the existence of a tunnel spontaneous transition from an energy level in shallow potential wells H^-- and D^-- into lower energy levels in Li^+-wells. In [4] it was proposed methods of interaction potentials calculation in (111) planes for an infinite crystal. On its basis in [5] it was made a revise account of potential wells in H^-- and D^--planes. Besides, it was shown that at T = 300 K in H^--planes there are shallow potential wells of ~ 0.3 eV depths vanishing at T = 600 K. The same fact is indicated in [6], where the calculation of potentials of electrons interaction with the charged (111) planes is realized on the basis of the methods proposed in [7] for a finite crystal. Besides, in [5] the identification of radiation transitions with experimental peaks different from the identifications in [2, 7] was made. To get more short-wave and more intensive short wave radiation (e.g. see spectral short wave dependencies for lithium halides crystals in [8]) in the given paper the analogous consideration for relativistic electrons with Lorentz-factors $\gamma = 50,\ 75,\ 100$ ($\varepsilon_{\|} \approx 25.6, 38.3, 51.1$ MeV) is carried out in the main charged [110] axes in LiH crystal at T = 300, 600, 900 K. It is necessary to note that channeling along the direction [110] is interesting because of the fact that in the charged Li^+ – [110] – axes, potential wells depths almost in 50% are formed by a long range Coulomb interaction with crystal ions and in the charged H^- – [110] – axes the inversion of potential wells into potential barriers occurs with temperature changing.

1. THE CALCULATION OF ELECTRON INTERACTION POTENTIALS WITH THE MAIN CHARGED [110] AXES IN HYDRIDE LITHIUM CRYSTAL AT DIFFERENT TEMPERATURES

Our analysis is based on the use of the following one-particle potentials for Li^+ and H^- ions in hydride lithium (LiH) crystal [9]:

$$\phi_+(r) = e\left[2\left(\frac{Z_+^*}{a_0}+\frac{1}{r}\right)\exp\left(-\frac{2Z_+^* r}{a_0}\right)+\frac{(1-\alpha)}{2a_0^3}\left(\frac{r^2}{4}+\frac{ra_0}{2}+\frac{3a_0^2}{2}+\frac{2a_0^3}{r}\right)\exp\left(-\frac{r}{a_0}\right)+\frac{\alpha}{r}\right], \quad (1a)$$

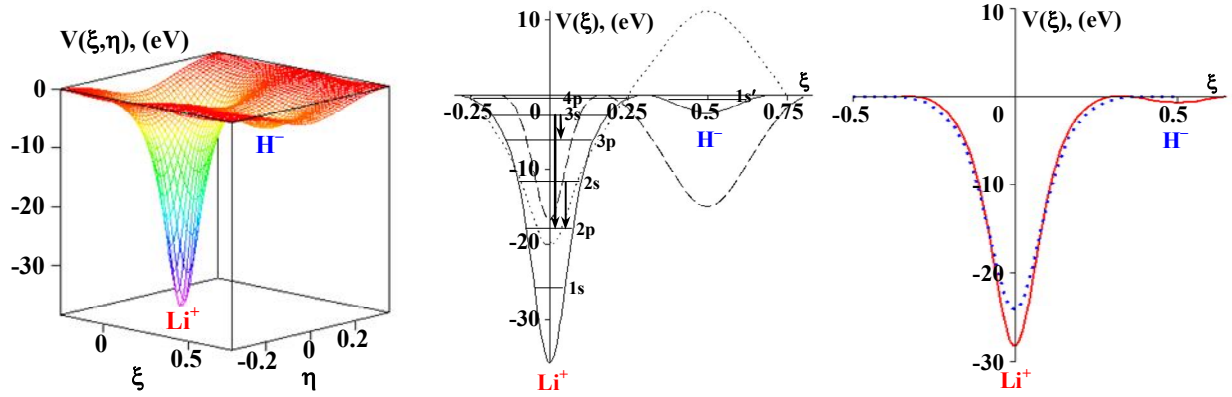
$$\phi_-(r) = e\left[(1+\alpha)\left(\frac{Z_-^*}{a_0}+\frac{1}{r}\right)\exp\left(-\frac{2Z_-^* r}{a_0}\right)-\frac{\alpha}{r}\right], \quad (1b)$$

where $Z_+^* e = 43e/16$ and $Z_-^* e = 11e/16$ – screened nuclei charges of Li^+ and H^- ions, correspondingly; α – the degree of ionicity of LiH crystal, which is estimated at 0.8 – 1 [3] (then select value 0.9); a_0 – the Bohr radius. After a standard procedure of a special averaging of both first two components in formula (1,a) and first component in formula (1,b) along the axes and an averaging by thermal oscillations (see, for example, [10]), we come to the following expressions for interaction potentials of electron with so-called electro-neutral skeletons, correspondingly, for main charged Li^+ and H^- axes [110] in LiH crystal:

$$V_+(\rho)=-\frac{2e^2}{d}\exp\left(-\frac{\rho^2}{2u_+^2}\right)\int_0^\infty s\exp\left(-\frac{s^2}{2}\right)I_0\left(\frac{\rho s}{u_+}\right)\left\{2K_0\left(\frac{2u_+Z_+^*}{a_0}\right)+\frac{2u_+Z_+^*}{a_0}K_1\left(\frac{2u_+Z_+^*}{a_0}\right)+\right.$$
$$\left.+\frac{(1-\alpha)}{8a_0^3}\left[K_0\left(\frac{u_+s}{a_0}\right)\left(3a_0u_+^2s^2+8a_0^3\right)+K_1\left(\frac{u_+s}{a_0}\right)\left(u_+^3s^3+10u_+a_0^2s\right)\right]\right\}ds\,, \qquad (2a)$$

$$V_-(\rho)=-\frac{2e^2(1+\alpha)}{d}\exp\left(-\frac{\rho^2}{2u_-^2}\right)\int_0^\infty s\exp\left(-\frac{s^2}{2}\right)I_0\left(\frac{\rho s}{u_-}\right)\left[K_0\left(\frac{2u_-Z_-^*}{a_0}\right)+\frac{u_-Z_-^*}{a_0}K_1\left(\frac{2u_-Z_-^*}{a_0}\right)\right]ds\,, \qquad (2b)$$

where $d=a/\sqrt{2}$ – a distance between ions along Li^+ and H^- axes (a – a constant of a crystal lattice); $u_\pm$ – an amplitude of thermal oscillations of these ions; $I_0(x)$ – a modified Bessel function; $K_{0,1}(x)$ – a MacDonald function. The calculation of interaction potentials of electron with the use of one-particle Coulomb components $\phi_\pm(r)=\pm\alpha e/r$ is realized in accordance with the methods proposed in [8, 11, 12]. In Fig. 1,a it is shown in relative $\xi=x/d$ and $\eta=y/d$ units in $(-1/4<\xi<3/4)\times\left(|\eta|<1/2\sqrt{2}\right)$ region of one two-dimensional period, 3D-plot of interaction potential of electron with all charged [110] axes. It is necessary to note that potential wells in charged Li^+ – [110] – axes are deeper comparing potential wells in main electro-neutral [100] and [111] axes in spite of the fact that mean densities of valence electrons in all these axes are similar. In the case of planar channeling, the potential wells in the main electro-neutral planes (100) are the deepest [2]. In Fig. 1,b in cross-section $\eta=0$ there are presented: 2D-plots of axial interaction potentials arising by taking into account interaction potentials (2a) and (2b) with the nearest Li^+ and H^- axes (a dashed curve); 2D-plot of Coulomb interaction potential with excess and missing charges of these axes (a dotted curve); 2D-plot of a summary interaction potential of electron with all charged [110] axes (a solid curve). All these potentials are calculated at T = 300 K. In Fig. 1,c summary interaction potentials at T = 600 K (a solid curve) and at T = 900 K (a dotted curve) are presented.



a *b* *c*

Fig. 1. 3D-plot of electron interaction potential with the main charged [110] axes in LiH crystal (a); 2D-plot of electron interaction potentials with electro-neutral skeletons of Li^+ and H^- axes (a dashed curve), with positive and negative charges of these axes (a dotted curve), and also a summary interaction potential (a solid curve), calculated at T = 300 K (b); 2D-plot of a summary interaction potential of electron with [110] axes at T = 600 K (a solid curve) and at T = 900 K (a dotted curve) (c)

From these data it is clear that for LiH crystal a contribution of a long range Coulomb interaction in a summary interaction potential is comparable with the contribution of electron interaction with electro-neutral skeletons of Li^+ and H^- axes. It means that along crystallographic Li^+ – [110] axes in LiH crystal, as in the charged (111) planes [4], quite deep potential wells arise at quite low valence electron density in these channels which leads to anomalous large lengths of relativistic electrons dechanneling. In H^- – [110] axes the depths of potential wells are small (see Fig. 1,c) and these depths tends to zero when crystal temperature is increased.

2. NUMERICAL CALCULATION OF TRANSVERSE ENERGY LEVELS AND CORRESPONDING WAVE FUNCTIONS

For the electrons with Lorentz-factors $\gamma = 50, 75, 100$ the transverse energy levels and corresponding wave functions in non-axial symmetric interaction potential of charged [110] axes of LiH crystals are calculated numerically. 3D-plot of this potential is presented in Fig. 1,a. This calculation was conducted in one two-dimensional period and in the approximation of axial symmetry for Li^+ and H^- axes. It is very important to note (see [10]) that at $\varepsilon_\parallel \geq 10$ MeV the "Bloch nature" of the motion of a fast charged particle in a periodic crystal potential can be ignored and the problem can be

solved within one isolated channel on the base of the following Schrödinger equation:

$$\left[\Delta_{\rho\varphi} - 2\mu\gamma\left[W(\rho) - \varepsilon_{n_\rho|m|}\right]/\hbar^2\right]\Phi_{n_\rho m}(\rho,\varphi) = 0. \quad (3)$$

The equation (3) after substitution $\Phi_{n_\rho m}(\rho,\varphi) = \frac{\rho^{|m|}}{\sqrt{2\pi}}\exp(im\varphi)\chi_{n_\rho|m|}(\rho)$ reduces to equation

$$\left\{-\frac{d}{d\rho}\left[p_m(\rho)\frac{d}{d\rho}\right] + q_m(\rho) - \lambda_{n_\rho m} r_m(\rho)\right\}\chi_{n_\rho|m|}(\rho) = 0, \quad (4)$$

which corresponds to the standard Sturm – Liouville problem. Here $m = 0, \pm1, \ldots$, $p_m(\rho) = r_m(\rho) = \rho^{2|m|+1}$, $q_m(\rho) = -2\mu\gamma W(\rho)\rho^{2|m|+1}/\hbar^2$, $\lambda_{n_\rho m} = 2\mu\gamma\varepsilon_{n_\rho|m|}/\hbar^2$.

The transverse energies $\varepsilon_{n_\rho|m|}$ and corresponding wave functions $\chi_{n_\rho|m|}(\rho)$ of equation (4) were calculated by means of the following program in IMSL Fortran 90 library accounting boundary condition $\chi_{n_\rho|m|}(\infty) = 0$. Besides, axial potentials were approximated by function $W(\rho) = -W_0/\cosh^\alpha(\rho/b)$ (for Li^+ axis $W_0 \approx 36$ eV, $b \approx 0.26$ A, $\alpha = 2$, and for H^- axis $W_0 \approx 2.6$ eV, $b \approx 0.9$ A, $\alpha = 15$).

Numerical values of the transverse energy $\varepsilon^{(\pm)}_{n_\rho|m|}$ for the channeling electrons with Lorentz-factors $\gamma = 50, 75, 100$ are given in Table. In this case all energy levels with $m = 0$ are *s*-levels and at $m = \pm1$ are *p*-levels [13].

Numerical values of transverse energy levels $\varepsilon^{(\pm)}_{n_\rho|m|}$ for electrons with Lorentz-factors $\gamma = 50, 75, 100$

γ	$-\varepsilon^{(\pm)}_{n_\rho\|m\|}$, eV							
	Li^+							H
	1s	2s	3s	4s	2p	3p	4p	1s′
50	24.71	8.14	0.55	-	14.96	2.97	-	0.65
75	26.57	11.72	2.87	-	18.16	6.36	0.61	0.89
100	27.73	14.19	5.08	0.55	20.21	8.94	2.19	1.06

As an illustration, in Fig. 1,b and Fig. 2,a,b transverse levels of energy $\varepsilon^{(\pm)}_{n_\rho 0}$ and $\varepsilon^{(+)}_{n_\rho 1}$ for $\gamma = 75$ and corresponding wave functions $\chi^{(\pm)}_{n_\rho 0}(\rho)$ and $\chi^{(+)}_{n_\rho 1}(\rho)$ are presented.

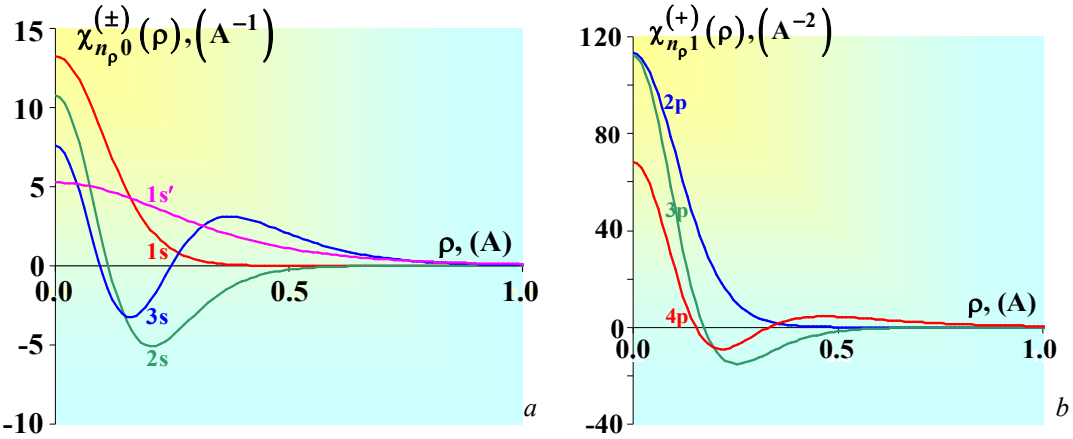


Fig. 2. Wave function plots arising at electron channeling with a Lorentz-factor $\gamma = 75$ along main charged Li^+ and H^- axes in LiH crystal correspondingly: at $m = 0$ (a); at $m = \pm1$ (b)

As seen from Fig. 1,a, in the near-barrier zone, the interaction potential is anisotropic. It contains potential ditches with ~ 2.5 eV depths, oriented along the *x*-axis. These channels are periodically located along the *y*-axis. It is known [10], that the width of these levels during axial channeling will be determined by inelastic scattering on the valence electrons of the crystal ions. Since the concentration of these electrons in Li^+ and H^- – axes is low, the widths of the transverse energy $\varepsilon^{(\pm)}_{n_\rho|m|}$ levels should be at least an order of magnitude lower than in the traditionally used covalent crystals and equal ~ 0.01 eV. This means that the lengths of dechannelings for the studied energy range will exceed 10 μm, which will contribute to obtaining sufficiently intense and monochromatic CR.

3. CALCULATION OF CR SPECTRA

The view of CR spectrum (per unit path length) of electron, moving at a small angle θ relative to the axis Li^+ – [110], will be calculated in accordance with the formula

$$G^{(+)}_\theta(\omega) = \frac{e^2\omega}{\hbar c^4}\sum_{n_\rho,m,n'_\rho,m'}\left|\vec{\rho}^{(+)}_{n_\rho m,n'_\rho m'}\right|^2\Omega^{(+)2}_{n_\rho|m|,n'_\rho|m'|}\times$$

$$\times f\left(\omega\Big/2\gamma^2\Omega^{(+)}_{n_\rho|m|,n'_\rho|m'|}\right)P^{(+)}_{n_\rho|m|}(\theta). \qquad (5)$$

This formula was obtained in the dipole approximation on the basis of [10] by analogy with the corresponding expressions in [8, 12]. Here

$$\left|\bar{\rho}^{(+)}_{n_\rho m,n'_\rho m'}\right|^2=\frac{1}{2}\left(\delta_{m',m+1}+\delta_{m',m-1}\right)\times$$

$$\times\left[\int_0^\infty \chi^{(+)}_{n_\rho|m|}(\rho)\chi^{(+)}_{n'_\rho|m'|}(\rho)\rho^{|m|+|m'|+2}d\rho\right]^2$$

is a module squared of the radial matrix element of the radiation transition between energy levels $\varepsilon^{(+)}_{n_\rho|m|}$ and $\varepsilon^{(+)}_{n'_\rho|m'|}$; $\Omega^{(+)}_{n_\rho|m|,n'_\rho|m'|}=\left[\varepsilon^{(+)}_{n_\rho|m|}-\varepsilon^{(+)}_{n'_\rho|m'|}\right]\Big/\hbar$ – frequency of transition between these levels; $P^{(+)}_{n_\rho|m|}=\frac{2\pi(2-\delta_{m0})}{A}\left|\int_0^\infty \rho^{|m|+1}\chi^{(+)}_{n_\rho|m|}(\rho)J_m(k_\perp\rho)d\rho\right|^2$ – the initial population of transverse energy levels $\varepsilon^{(+)}_{n_\rho|m|}$ (see, e.g. [13]), $k_\perp\approx\mu c\gamma\left(1-1/2\gamma^2\right)\theta/\hbar$, $A=a^2/2\sqrt{2}$ – the area of two-dimensional period, $J_m(x)$ – m-th order Bessel function; $f(x)=(1-2x+2x^2)\theta(1-x)$. Here δ_{mn} denotes the Kronecker delta, $\theta(x)$ – Heaviside function. The spectral distributions $G^{(+)}_\theta$ for a dispersionless beam of relativistic electrons with Lorentz-factors $\gamma=50, 75, 100$, moving under a zero angle regarding Li^+ – [110] axes is presented in Fig. 3,a. In this case, as it follows from the expression for $P^{(+)}_{n_\rho|m|}$, only energy levels with $m=0$ are populated. Because of this reason there are only few spectral peaks (for example, three peaks at $\gamma=75$, corresponding to transitions $3s\to3p$, $2s\to2p$, and $3s\to2p$, which are shown in Fig. 1,b. In the case of an electron beam with a certain angular dispersion θ_0, when calculating the emission spectrum, it is necessary to use the initial population in the formula (5), averaged by means of a normal distribution function $g(\theta)=\left(2\pi\theta_0^2\right)^{-1/2}\exp\left(-\theta^2/2\theta_0^2\right)$. Fig. 3,b presents spectral CR $\left\langle G^{(+)}_\theta(\omega)\right\rangle_{\theta_0}$ for electron beams, for example, with $\gamma=75$ and with $\theta_0\approx0.5$, 1, 2 mrad angular dispersions.

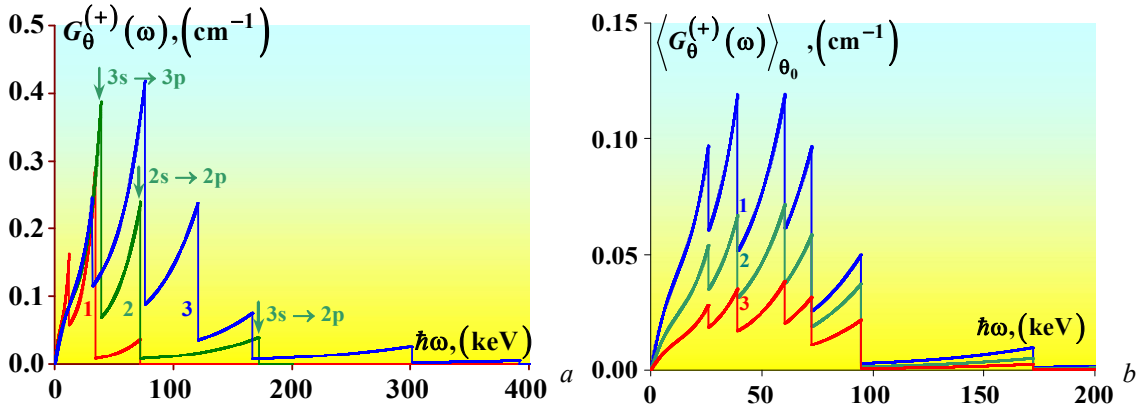


Fig. 3. Spectral distributions of CR electron energy on a unit path at its motion under a zero angle to Li^+ – [110] axes of LiH crystal (the calculations are made for a Moliere approximation): for dispersionless electron beams with Lorentz-factors $\gamma=50$ (curve 1), $\gamma=75$ (curve 2), $\gamma=100$ (curve 3) (a); with electron beams with a Lorentz-factor $\gamma=75$ at angular dispersions $\theta_0\approx0.5$ mrad (curve 1), $\theta_0\approx1$ mrad (curve 2), $\theta_0\approx2$ mrad (curve 3) (b)

As can be seen from Fig. 3,b, for an electron beam with non-zero angular dispersion, moving at zero angle to the Li^+ – [110] axes, the spectral distributions essentially change: a) the number of peaks is doubled, since now the levels with $m=\pm1$ are also populated; b) the spectral peak values decrease slightly at the same total intensity; c) the spectral distribution becomes more uniform in a narrower spectral range.

CONCLUSIONS

In the work there were calculated the interaction potentials of electrons with the main charged [110] axes in LiH crystal. It was shown that a Coulomb interaction contributes considerably into potential wells depth in Li^+ axes. It is shown also that in H^- axes the inversion of potential wells into barriers arises at a certain temperature.

For relativistic electrons with Lorentz-factors $\gamma=50$, 75, 100 transverse energy levels and their corresponding wave functions are calculated numerically. There were found the widths of these levels by means of which dechanneling lengths are evaluated.

In the frames of a dipole approximation for electron beams with different angular dispersions there were found spectral distributions of CR energy demonstrating the possibility of quite intensive short-wave radiation obtaining.

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ОСОБЕННОСТИ КАНАЛИРОВАНИЯ И ГЕНЕРИРУЕМОГО ИЗЛУЧЕНИЯ РЕЛЯТИВИСТСКИХ ЭЛЕКТРОНОВ В ЗАРЯЖЕННЫХ ОСЯХ КРИСТАЛЛА ГИДРИДА ЛИТИЯ

Н.В. Максюта, В.И. Высоцкий, С.В. Ефименко, Ю.А. Слинченко

Произведен расчет потенциалов взаимодействия электронов с главными заряженными осями [110] в кристалле гидрида лития при температурах T = 300, 600 и 900 K. Для релятивистских электронов с Лоренц-факторами γ = 50, 75, 100 численно найдены энергии и соответствующие им волновые функции поперечных уровней каналированного движения. На основе этих данных рассчитаны спектры излучения каналируемых электронов с учетом (и без учета) угловой дисперсии.

ОСОБЛИВОСТІ КАНАЛЮВАННЯ ТА ГЕНЕРОВАНОГО ВИПРОМІНЮВАННЯ РЕЛЯТИВІСТСЬКИХ ЕЛЕКТРОНІВ У ЗАРЯДЖЕНИХ ОСЯХ КРИСТАЛА ГІДРИДУ ЛІТІЮ

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Проведено розрахунок потенціалів взаємодії електронів із головними зарядженими осями [110] у кристалі гідриду літію за температур T = 300, 600 і 900 K. Для релятивістських електронів із Лоренц-факторами γ = 50, 75, 100 чисельно знайдені енергії та відповідні їм хвильові функції поперечних рівнів канальованого руху. На основі цих даних розраховано спектри випромінювання канальованих електронів за врахуванням (та без врахування) кутової дисперсії.