Polarization and correlation aspects of resonant coherent excitation of fast highly charged ions in crystals

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Abstract. We report selected results of our latest calculations on polarization properties of the in-crystal resonating electric field and their manifestation in the yield, angular distribution and polarization parameters of the characteristic X-ray radiation from resonant coherent excited relativistic highly charged ions under planar channeling.

1. Introduction
Unambiguous observation of resonant coherent excitation (RCE) of channeled ions in crystals made by S.Datz group three decades ago [1] and, now, the comprehensive experiments performed by the Tokyo RCE collaboration using relativistic highly charged ion beams (see their latest publication [2] and references therein) revert us to fundamental predictions made in 1965 by V.V.Okorokov [3] and to his pioneer experimental and theoretical studies on this phenomenon. The Okorokov effect appears when one of the harmonics of the spatially periodic electric field of the crystal acts on the moving ion with a resonance frequency corresponding to the ion excitation energy. The anisotropic character of the field manifests itself in the produced alignment (angular momentum polarization) of the excited ions and, hence, in possible angular anisotropy, linear polarization and, under special conditions, circular polarization of their characteristic X-ray radiation.

Our theoretical studies link together the origin and the wide set of observables of the RCE process. Treating the propagating ion as an open quantum system involved into both coherent and incoherent (relaxation) interactions with its environs, they are based of a unified concept [4] of the generalized Master equation description of the time evolution of the excitation and decay properties of the propagating ions together with the well-known density matrix (statistical tensors) technique to deal with polarization and correlation phenomena in atomic collisions [5]. Our recent calculations suggest a quantitative theoretical analysis of such fundamental RCE experiments by the Tokyo group as observation of the axial symmetry violation in the angular distribution of the X-rays from planar channeled resonant coherently excited relativistic Fe$^{24+}$ ions in Si crystal [6, 7], first double-resonant excitation of ionic autoionizing states [8, 9], a comprehensive analysis of recent observation of the Autler-Townes doublet in resonant coherent excitation of the helium-like ions in crystals beyond the channeling conditions [2, 10, 11] and, also in the non-channeling conditions, fine structure of resonances in relativistic hydrogen-like ions [11, 12]. At the same time a number of new aspects of the RCE studies has been
considered and modelled by computer simulation for corresponding future experiments. They concern the yield and angular anisotropy of the Auger electrons produced by resonant coherent excitation of relativistic highly charged ions in channeling and non-channeling conditions [9,11], the metastable ion production in the RCE process [13, 14], the trajectory resolved X-ray measurements in this process in the ion – X-ray coincidence experiments [14] and others.

A compact presentation of our approach together with main results of its application was given at the conference HCI2008 [14]. Supplementing it by our new calculations, we concentrate here on one special aspect of the problem strictly corresponding to the subject (of the second part) of the Symposium to draw a line from polarization properties of the resonating field of the crystal acting on the ion to the angular anisotropy and polarization properties of the characteristic X-ray radiation in the RCE process including possible perspectives of its applications.

2. From spectral and geometrical properties of the resonating electric field of the crystal to the Stokes parameters of the RCE ion characteristic X-ray radiation

In paper [15] on the RCE process with planar channeled ions, we showed that taking a special coordinate axes and, also, using the dipole approximation to represent the crystal electric field in the ion rest frame one reaches considerable advantages to parameterize the excited ion density matrix and, hence, to consider the angular distribution of the photons in both cases of trajectory resolved and non-resolved RCE measurements. On this way, we revealed that the field in the ion rest frame is elliptically polarized but its opposite circulation in the upper and the lower parts of the channel compensate the produced vector polarization of the whole ensemble of the excited ion when they enter the channel symmetrically according to standard conditions of the RCE experiments. Therefore, according to general symmetry rules, the observation of circularly polarized photons in all these RCE experiments is strictly forbidden.

This is not so as concerns tensor polarization (alignment) of the excited ions and, hence, angular anisotropy and linear polarization of the radiation where both parameters are determined by the same set of statistical tensors of rank 2 of the excited ion. In Fig.1 we reproduce our calculation [7] for the first unambiguous observation of the alignment effect in the RCE process made by the Tokyo group [6] with 423 MeV/u Fe$^{24+}$ ion in the (220) planar channel in Si crystal. Contrary to the case of RCE of light channeled ions of relatively low energies where the Okorokov effect is concentrated, due to strong relaxation processes near the channel walls, only in a very narrow central part of the channel [16], here the corresponding coherence zone turns out to be on the level of about 90%.

**Figure 1.** Differential yield of the X-ray radiation as a function of the crystal rotation angle $\theta$ at $(k, l) = (2, -1)$ for 423 MeV/u Fe$^{24+}$ ion in 21 $\mu$m Si crystal, measured in [6] and calculated in [7] for two directions: in the channeling plane (white squares — experiment, solid line — calculation) and perpendicular to the channel (black circles — experiment, dashed line — calculation). Inset shows calculation results in the same conditions for the major peak of $(k, l) = (1, 3)$ resonance.
2.1. Our calculation procedure (briefly)

Scalar potential \( \varphi(\vec{r}) \) of the electric field of the crystal is composed in the laboratory frame into its Fourier \((kln)\) harmonics

\[
\varphi(\vec{r}) = \sum_{kln} \Phi_{kln} e^{i\vec{G}_{kln}\cdot\vec{r}},
\]

with wave vectors \( \vec{G}_{kln} \) being reciprocal lattice vectors. After a set of successive coordinate frame transformations this potential is transformed into the the scalar and vector electromagnetic potentials in the ion rest frame:

\[
\varphi'(\vec{r}', t') = \gamma \sum_{kln} e^{i\vec{G}_{kln}\cdot\vec{r}'} \Phi_{kln} e^{\pi i n/z_{\text{ion}} / d + 1/2} e^{i\vec{G}_{kln}\cdot\vec{r}'},
\]

\[
\vec{A}'(\vec{r}', t') = -\vec{e}_x \frac{\gamma v}{c} \sum_{kln} e^{i\vec{G}_{kln}\cdot\vec{r}'} \Phi_{kln} e^{\pi i n/z_{\text{ion}} / d + 1/2} e^{i\vec{G}_{kln}\cdot\vec{r}'},
\]

with vectors \( \vec{G}'_{kln} = \vec{G}_{kln} + (\gamma - 1)(\vec{G}_{kln})_x \vec{e}_x \) standing for the reciprocal lattice vectors in the ion rest frame, which \( x \)-component is \( \gamma \) times larger, due to relativistic lattice contraction, than \( x \)-component of \( \vec{G}_{kln} \). Hamiltonian \( H_0 \) of the free ion and the operator

\[
V = -e \varphi' + \frac{e}{2mc}(\vec{p}\vec{A}' + \vec{A}'\vec{p})
\]

of its interaction with the potentials \( \varphi'(\vec{r}', t') \) and \( \vec{A}'(\vec{r}', t') \) form the total Hamiltonian of the channeled ion \( H = H_0 + V \) entering the generalized Master equation

\[
\frac{i}{\hbar} \frac{\partial \rho}{\partial t} = [H, \rho] + R\rho,
\]

which describes time evolution of the density matrix \( \rho \) of the ion. The spin-orbit interaction is included in \( H_0 \). Time dependence of the field acting on the ion, expressed by the first exponents in (2), leads to the Okorokov resonance condition between the field frequency and the ion transition energy \( E_{\text{trans}} \):

\[
\frac{2\pi \gamma v}{a} (k \sqrt{2} \cos \theta + l \sin \theta) = E_{\text{trans}}.
\]

Indices \((k, l)\) represent a family of the reciprocal lattice vectors \( \vec{G}_{kln} = \vec{G}_{k0l} + \vec{G}_{0ln} \) with various \( n \) values. All they have the same \( \vec{G}_{k0l} \) component lying in the channel plane but different perpendicular to the channel \( \vec{G}_{0ln} \) components. Solving equation (4) numerically in a chosen basic of states of a free ion, we project density matrix \( \rho(t) \) on the subspace of the ion states emitting photons (say, states \( 2^l P_1 \) in case of RCE of helium-like ions) and transform this submatrix \( \rho^{(\gamma)}(t) \) into its statistical tensors to use standard methods of calculating angular distribution and polarization of the radiation.

2.2. Elliptically polarized electric field of the crystal in the ion rest frame

Following [15] consider the resonant \((k,l)\) term

\[
E_{kl}'(\vec{r}', t') = -i \gamma e^{i\vec{G}_{k0l} \cdot \vec{r}'} \sum_n G_{kln}^{\mu} \Phi_{kln} e^{\pi i n/z_{\text{ion}} / d + 1/2} e^{i\vec{G}_{kln}\cdot\vec{r}'}
\]

of the vector of the electric field strength \( E'(\vec{r}', t') = -\nabla_{\vec{r}'} \varphi' - (1/c)(\partial \vec{A}' / \partial t') \) acting upon the ion in its rest frame. It is a superposition of the components directed along auxiliary vectors

\[
G_{kln}^{\mu} = \delta_{kln} - \frac{\gamma - 1}{\gamma} (\vec{G}_{kln})_x \vec{e}_x,
\]
where their $y$- and $z$-components are the same as those of corresponding $\vec{G}_{kln}$ vectors but $x$-components are $\gamma$ times smaller. All vectors $\vec{G}_{kln}'$ with fixed $(k, l)$ lie in the same plane which is perpendicular to the channel plane and crosses it on the line directed along the vector $\vec{G}_{kl0}'$.

To reveal the elliptic character of the oscillating electric field of the crystal, take a special ion rest frame $(X,Y,Z)$ with $X$ axis directed towards $\vec{G}_{kl0}'$ and $Z$ axis is perpendicular to the channel plane and consider a general case of resonant coherent excitation of $1s^2: 1S_0 \rightarrow 1s2p: 1P_1$ transition in helium-like ions in $(2\overline{2}0)$ planar channel. Then, using the dipole approximation, reduce operator (3) to scalar product of the ion electric dipole moment operator $\vec{d}_{\text{ion}}$ and the strength of the field $\vec{E}_{kl}(0, t')$ at the ion nucleus: $V^{(\text{dip})}(t') = -\vec{d}_{\text{ion}} \vec{E}_{kl}(0, t')$.

In [15], we showed that the phase shift between time oscillations of the $[\vec{E}_{kl}(0, t')]_X$ and $[\vec{E}_{kl}(0, t')]_Z$ Cartesian components of the field $\vec{E}_{kl}(0, t')$ in the ion rest frame $(X,Y,Z)$ is $\pm \pi/2$ at any position $z_{\text{ion}}$ of the ion in the channel. The ellipse of this rotating field lies in $(X,Z)$ plane and its axes are directed along $X$ and $Z$ coordinate axes (Fig.2). The specific character of the resonating crystal field can produce vector polarization of the trajectory resolved RCE ions which, in turn, can be revealed by detecting their X-ray photons in coincidence with those of the ions whose trajectories lie on one side relative to the central channel plane [14]. Their selection can be performed when the target thickness is of the quarter of the period of the ion transverse oscillations between the walls of the channel (such a procedure was previously used in experiment [17] when measuring the charge state distribution of the RCE ions).

2.3. Stokes parameters of the X-ray radiation from the RCE ions in the laboratory frame

In [18] we presented the total set of the Stokes parameters of the X-rays from resonant excited 423 MeV/u Fe$^{24+}$ ions in the $(2\overline{2}0)$ planar channel of the Si crystal; its 21-$\mu$m target

![Figure 2. Schematic illustration of the elliptically polarized field of the crystal and polarization characteristics of the photons repeating the geometrical properties of the ellipse in various emission directions.](image)

![Figure 3. Angular distribution (solid line, in arbitrary units) of the yield and linear polarization degree $P_L$ (dotted line) of photons emitted over the cone with the photon deflection angle 43.5° in the laboratory frame for 423 MeV/u Fe$^{24+}$ beam in the 21-µm-thick target (in the ion rest frame these photons are emitted perpendicularly to the beam). Dashed line shows the circular polarization degree $P_3$ calculated for the 0.9-µm-thick target with averaging over one half of the channel.](image)
thickness was taken according to the experiment [6]. Here, the energy $E_{tr} = 6.7$ keV of the $1s^2p^4 \rightarrow 1s^2p^2$ transition varies in the laboratory frame from 2.75 to 16.82 keV. Note, first of all, a large angle-integrated radiation yield; at the resonance maximum, it is 1.8 photons per incident ion.

Angular distribution $W(\theta_\gamma, \phi_\gamma)$ of photons and their Stokes parameters $P_1$, $P_2$ and $P_3$ are first calculated directly from the submatrix $\rho^{(\gamma)}$ and its statistical tensors $\phi^{(\gamma)}_{kq}$ in the ion rest frame and then are transformed into the lab-frame according to the usual Lorentz transformation rules. Fig.3 presents an example of the results of these calculations. They demonstrate possibilities to vary the frequency of the resulting radiation and select its polarization characteristics in a wide range. An extension of our circular polarization suggestions to such an RCE experiment layout in which the ion beam entering the target is slightly inclined relative to the channel plane is in progress.

3. Conclusion

We have built a continuous line of theoretical description of the RCE process from the basic polarization properties of the resonating in-crystal electric field to the yield, angular distribution and polarization parameters of the characteristic X-ray radiation from resonant coherent excited highly-charged ions under planar channeling in crystals. The calculations show that since the photon yield and their polarization parameters in conditions typical or close to current RCE experiments are expected to be large, the resonance coherent excitation method can, indeed, be considered as a candidate for a tunable source of polarized X-ray radiation in the keV region [6].

Acknowledgments

Author appreciates his customary collaboration on various aspects of the RCE studies with I. Bodrenko, A. Sokolik, A. Stysin and V. Dolinov. The work was supported by RFBR (grants 08-02-08690, 09-02-01266).

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