



Angular anisotropy of the RCE X-rays under planar channeling as manifestation of geometric properties of the in-crystal electric field

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ABSTRACT

Planar channeled ion under resonant coherent excitation conditions experiences an action of the oscillating electric field arising in the ion rest frame. We show how the alignment of the angular momentum of coherently excited ions and, hence, the angular anisotropy of their characteristic X-ray radiation are connected with the geometrical and symmetry properties of this field. The consideration is based on two examples of $(k, l) = (2, -1)$ and $(1, 3)$ resonances with 423 MeV/u Fe^{24+} ions in $(2\bar{2}0)$ planar channel of Si crystal, corresponding to different symmetries of the resonant field. In both cases the resonant electric field is elliptically polarized. A choice of an appropriate coordinate frame allows us to show the connection between the geometrical properties of the resonant field and the X-ray angular distributions especially clear. To illustrate, we calculate angular distributions of X-rays for individual ionic trajectories using density matrix formalism and then consider formation of the angular distributions not resolved by ion trajectory. Comparison with recent experimental data is done.

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1. Introduction

Resonant coherent excitation (RCE) of swift ions under channeling conditions occurs when one of spatial harmonics of the in-crystal electric field acts on a bound electron of the ion with a resonant frequency corresponding to its excitation energy (see [1] and references therein). The resonantly excited ions then decay via two competing channels: collisional ionization and radiative deexcitation. This suggests two ways to observe RCE experimentally: (1) by measuring charge-state distribution of the transmitted ions and (2) by registration of characteristic X-ray radiation. An increase of the characteristic X-ray yield under RCE conditions was unambiguously observed in [2–4]. Angular anisotropy of the X-rays distribution was first reported in [5] for Mg^{11+} ions at 25 MeV/u in (100) planar channel of Ni crystal. In the series of experiments on RCE of relativistic heavy ions [6] the X-ray radiation resonant profile [7] and slight anisotropy of this radiation [8] were measured for 390 MeV/u Ar^{17+} in $(2\bar{2}0)$ planar channel of silicon. Recently, very strong anisotropy was reported [9] for 423 MeV/u Fe^{24+} helium-like ions in the same channel.

Angular anisotropy of the X-ray radiation indicates that electron cloud of the ion is aligned during excitation by the electromagnetic

field of crystal. Theoretically, the ion excitation–deexcitation cascade is most conveniently treated in the ion rest frame. Here we take into account both scalar and vector potentials of the electromagnetic field arising in the moving frame and show, how certain geometrical and symmetry properties of the electric field manifest in the characteristic features of the ion excitation and, hence, in the angular distribution of its X-ray radiation. In the framework of the dipole approximation, this connection becomes especially clear. Calculations illustrating the theoretical consideration are performed by means of the density matrix formalism, which was successfully used to describe the experimental results on RCE of both non-relativistic [10–12] and relativistic [13,14] ions. Being motivated by the recent RCE experiments involving trajectory resolved measurements [15], we consider angular distributions of X-rays corresponding to individual ion trajectories and then treat a sum of such trajectory resolved components as an X-ray distribution, not resolved by ion trajectory.

Two specific examples close to conditions of recent experiments [9] are considered. In both of them Fe^{24+} helium-like ions at 423 MeV/u are moving in $(2\bar{2}0)$ planar channel of Si crystal. The case of $(k, l) = (2, -1)$ resonance of the experiment [9] is analyzed theoretically in parallel with the case of $(k, l) = (1, 3)$ resonance in the same conditions. Both resonances have similar intensities but are quite different (as will be shown below) with respect to the geometrical properties of the corresponding electric field.

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For the considered Fe^{24+} ion RCE occurs through dipole $1s^2 : ^1S_0 \rightarrow 1s2p : ^1P_1$ transition. Due to the spin–orbit coupling and Stark mixing by the Lindhard potential the states $1s2s : ^1S_0$ and $1s2p : ^3P_1$ are also excited via $1s2p : ^1P_1$ state. In the experiment [9] two resonant peaks in X-rays yield were observed. The minor peak at $E_{\text{trans}} \approx 6667.5$ eV corresponds, according to our calculations, to the excitation of a mixture of $1s2s : ^1S_0$, $1s2p : ^1P_1$ and $1s2p : ^3P_1$ states. The major peak at $E_{\text{trans}} \approx 6700.4$ eV is due to the excitation of $1s2p : ^1P_1$ and $1s2p : ^3P_1$ states mixed in the proportion of about 9:1. It is the latter peak that demonstrates large anisotropy of X-ray emission and is addressed in our consideration.

The paper is organized as follows. In Section 2, we describe the in-crystal electromagnetic field acting on the ion and show its elliptically polarized character in the ion rest frame. Specially chosen coordinate system allows us to present the geometrical properties of the resonant component of the field in a particularly simple form. In Section 3, we consider trajectory resolved angular distributions of X-ray photons from the ions excited by the resonant field and present the results of our calculations. In Section 4, we discuss a formation of the total X-ray angular distribution, not resolved by ion trajectories, and Section 5 concludes the paper.

2. Channeled ion excitation by the resonant electric field

2.1. The resonating field in the ion rest frame

Due to periodicity of crystal lattice, the scalar potential of the electric field inside the crystal in the laboratory frame may be represented as a composition of plane waves,

$$\varphi(\vec{r}) = \sum_{kln} \Phi_{kln} e^{i\vec{G}_{kln}\vec{r}}, \quad (1)$$

with their wave vectors $\vec{G}_{kln}$ being reciprocal lattice vectors. To consider channeling in $(2\bar{2}0)$ planar channel we, following [6], choose the crystal-bound coordinate system with X' , Y' and Z' axes set along the $[110]$, $[001]$ and $[1\bar{1}0]$ crystallographic directions respectively (thus $(2\bar{2}0)$ channeling plane coincides with (X', Y') plane). In this system

$$\vec{G}_{kln} = \frac{2\pi}{a} \{ k\sqrt{2}\vec{e}_{X'} + l\vec{e}_{Y'} + n\sqrt{2}\vec{e}_{Z'} \}, \quad (2)$$

where $a = 5.43$ Å is the lattice constant. The coefficients $\Phi_{kln} = \Phi(|\vec{G}_{kln}|)f_{kln}$, where $\Phi(G)$ depends on details of the electric potential distribution produced by a single target atom, and the geometrical structure factors for the diamond-like silicon lattice are

$$f_{kln} = 2 \left[1 + (-1)^{k+l+n} \right] \left[1 + (-i)^{2k+l} \right]. \quad (3)$$

We use Doyle–Turner relativistic Hartree–Fock results [16] to calculate $\Phi(G)$.

At fixed energy of the ion beam, tuning on a certain (k, l) resonance is realized by rotating the target over the normal to the channel plane, thereby we denote the angle between the ion beam and X' axis as θ . It is convenient, similarly to [6], to switch from the coordinate system (X', Y', Z') to another one (x, y, z) by doing the rotation on this angle in the (X', Y') plane so as to direct x axis along the beam, with z axis directed along $[1\bar{1}0]$. In this coordinate system the reciprocal lattice vectors (2) are

$$\vec{G}_{kln} = \frac{2\pi}{a} \left\{ (k\sqrt{2}\cos\theta + l\sin\theta)\vec{e}_x + (-k\sqrt{2}\sin\theta + l\cos\theta)\vec{e}_y + n\sqrt{2}\vec{e}_z \right\}. \quad (4)$$

To account for the action of the electric field on the ion moving with relativistic velocity v one switches to the ion rest frame $(\vec{r}', t')$ by means of the Lorentz transformations

$$x = \gamma(x' + vt'), \quad y = y', \quad z = z' + z_{\text{ion}}, \quad t = \gamma(t' + vx'/c^2), \quad (5)$$

$$\varphi'(\vec{r}', t') = \gamma\varphi(\vec{r}, t), \quad \vec{A}'(\vec{r}', t') = -\vec{e}_x(\gamma v/c)\varphi(\vec{r}, t), \quad (6)$$

where $\gamma = (1 - v^2/c^2)^{-1/2}$ is the Lorentz factor and z_{ion} is the ion transverse coordinate in the planar channel measured from the channel center ($\vec{r}'$ is now measured from the ion nucleus). Substituting these transformations into (1) and using (4), we obtain the scalar and vector electromagnetic potentials in the ion rest frame:

$$\begin{aligned} \varphi'(\vec{r}', t') &= \gamma \sum_{kln} e^{i\gamma v t' (\vec{G}_{kln})_x} \Phi_{kln} e^{\pi i n (z_{\text{ion}}/d + 1/2)} e^{i\vec{G}_{kln}\vec{r}'}, \\ \vec{A}'(\vec{r}', t') &= -\vec{e}_x \frac{\gamma v}{c} \sum_{kln} e^{i\gamma v t' (\vec{G}_{kln})_x} \Phi_{kln} e^{\pi i n (z_{\text{ion}}/d + 1/2)} e^{i\vec{G}_{kln}\vec{r}'}. \end{aligned} \quad (7)$$

Here $d = a/2\sqrt{2}$ is the channel width, and the vector

$$\vec{G}'_{kln} = \vec{G}_{kln} + (\gamma - 1)(\vec{G}_{kln})_x \vec{e}_x$$

is the reciprocal lattice vector in the ion rest frame, which x -component is γ times larger, due to relativistic lattice contraction, than x -component of $\vec{G}_{kln}$, whereas y - and z -components are the same.

The Hamiltonian H_0 of the free ion and the operator

$$V = -e\varphi' + \frac{e}{2mc} (\vec{p}\vec{A}' + \vec{A}'\vec{p}) \quad (8)$$

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 [17]

$$i\frac{\partial \rho}{\partial t} = [H, \rho] + R\rho, \quad (9)$$

which describes time evolution of the density matrix ρ of the ion (we neglect in (8) the term of magnetic field interaction with the electron spin and second-order interaction terms owing to smallness of the external field compared to the inter-ionic one). The operator R is responsible for the relaxation processes, caused by incoherent ion interactions with its surroundings, and by the spontaneous radiative deexcitation of the ionic excited states. In our case the differential Eq. (9) is solved numerically for the density matrix ρ expressed in the interaction representation in a basis of 8 states of helium-like Fe^{24+} ion taken in the LS coupling scheme: the ground state $1s^2 : ^1S_0$ and the excited states $1s2s : ^1S_0$, $1s2p : ^1P_{1,M}$ and $1s2p : ^3P_{1,M}$ with different projections M of the total momentum. The spin–orbit interaction is included in H_0 .

Time dependence of the field acting on the ion, expressed by the first exponents in (7), leads to the resonance condition, i.e. the condition of equality between the field frequency and the ion transition energy E_{trans} :

$$\frac{2\pi\gamma v}{a} (k\sqrt{2}\cos\theta + l\sin\theta) = E_{\text{trans}}. \quad (10)$$

The pair of indices (k, l) represents a family of the reciprocal lattice vectors with various n values. All these vectors $\vec{G}_{kln} = \vec{G}_{kl0} + \vec{G}_{00n}$ have the same $\vec{G}_{kl0}$ component lying in the channel plane but different perpendicular to the channel $\vec{G}_{00n}$ components. Their interference leads to dependence of the electromagnetic field on the transverse coordinate across the channel. By tuning on a certain (k, l) resonance one effectively exposes the ion to the corresponding components φ'_{kl} and $\vec{A}'_{kl}$ of the field (7). Usually, all other components do not influence ion excitation due to their rapid oscillations [18]. The only exception is the component $(k, l) = (0, 0)$ of φ' representing the Lindhard continuous potential which keeps the ion within the channel and causes Stark mixing of ionic excited states.

Hereafter we shall work in the ion rest frame and consider the resonant component of the field for a chosen (k, l) resonance. We introduce the vector of the electric field strength

$$\vec{E}'(\vec{r}', t') = -\nabla_{\vec{r}'}\varphi' - (1/c)(\partial\vec{A}'/\partial t') \quad (11)$$

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