Stark mixing of ionic intermediate states in radiative recombination of channeled ions

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Abstract. Stark mixing of intermediate excited ionic states due to combined action of crystal lattice, polarization wake potential and collisions with electrons is considered theoretically. Calculations for radiative recombination of well-channeled Ar and Kr ions under planar channeling in Si crystal show significant influence of the mixing of $|n = 2\rangle$ states on formation of the X-ray spectra and angular correlation between L-REC and K$\alpha_1$ photons.

1. Introduction
Radiative electron capture (REC) by channeled ions [1, 2] takes place under non-central ion-target interactions inducing specific processes in the electron shell of the propagating ion via Stark mixing of its excited states. We suggest a unified approach to investigate theoretically both aspects of this mixing: a) due to the combined crystal lattice and polarization wake potential (the field mixing); b) due to ion collisions with free electrons in the channel, leading, in parallel with electron loss and electron capture processes, to state-to-state transitions in the ion electron shell (the collisional mixing). Our goal is to reveal the relationships of these mechanisms to REC observables, known according to recent experimental studies in the field or suggested on the basis of calculations for future experiments. Our special interest concerns theoretical grounds for coincident REC measurements with channeled ions. As a whole, the present work is based on the density matrix approach [3, 4] to treat the channeled ion as an open quantum system involved into coherent and incoherent interactions with its surrounding and, on the other hand, on formalism [5, 6] describing polarization and correlation phenomena in recombination processes. Our approach is purely nonrelativistic.

Throughout the paper we consider a case of planar channeling of hydrogen-like ions produced in radiative electron capture by incoming bare nuclei. REC studies with planar channeled ions may be of special interest from both theoretical and experimental points of view as the breakdown of axial symmetry of interaction of ion beam with matter is much more pronounced here than in case of axial channeling.

2. The density matrix approach and REC observables
We consider the ion density matrix $\rho_{pq}(t)$ in the representation of $|n = 1\rangle$ and $|n = 2\rangle$ eigenstates $|p\rangle$ of the total Hamiltonian of the bound electron

$$\hat{H}_{\text{ion}} = \hat{H}_{\text{ion}}^{\text{free}} + \hat{V}_{\text{lattice}} + \hat{V}_{\text{wake}},$$

(1)
which includes the continuous (Lindhard) potential of the lattice $V_{\text{lattice}}$ and the polarization wake potential $V_{\text{wake}}$. Both last terms and, hence, the whole Hamiltonian (1), together with its eigenvalues $E_p$ and eigenvectors $|p\rangle$, depend on ion location $r_{\text{ion}}$ in the channel and, due to the curvilinear character of the ion trajectory, they are time-dependent.

The generalized master equation [7] for the density matrix $\hat{\rho}(t)$

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\hat{H}_{\text{ion}}, \hat{\rho}] + \hat{R}\hat{\rho},$$

where the relaxation operator $\hat{R}$ is responsible for incoherent processes of ion bound electron interaction with its environment in the channel, is solved as a system of coupled equations for matrix elements of $\hat{\rho}(t)$ in the representation of basic states $|p\rangle$ with time-dependent rate coefficients. The initial condition $\rho_{pq}(0) = \delta_{p0}\delta_{q0}$ corresponds to the case of target bombarded by a beam of bare nuclei.

2.1. Observables from single-detector measurements

The yield and angular distribution of L-REC photons, emitted at a fixed point $r_{\text{ion}}$, summed over corresponding group $\{p\}_{L-\text{REC}}$ of produced states and integrated over whole ion trajectory beginning at the entrance transverse coordinate $x_0$ are calculated as

$$\frac{dY_{L-\text{REC}}}{dx_0} = \int_0^{t_{\text{out}}} dt \sum_{p \in \{p\}_{L-\text{REC}}} \langle p, k_\gamma | \hat{O}_{\text{REC}} | 0, k_\gamma \rangle \rho_{00}(t) \langle 0, k_\gamma | \hat{O}^+_{\text{REC}} | p, k_\gamma \rangle,$$

where $\rho_{pq}(t)$ stands for fraction of bare nuclei in the beam. Calculation for K-REC is similar.

The yield and angular characteristics for K$_{\alpha_1}$ and K$_{\alpha_2}$ or for K$_\alpha$ photons as a whole are determined by corresponding groups $\{p\}_{K_{\alpha_1}}$, $\{p\}_{K_{\alpha_2}}$ and $\{p\}_{K_{\alpha}}$ of emitting ionic states, selected by the X-ray detector according to their excitation energy. For example, the differential yield of K$_{\alpha_1}$ radiation for the whole trajectory is calculated as

$$\frac{dY_{K_{\alpha_1}}}{dx_0} = \int_0^{t_{\text{out}}} dt \sum_{p \in \{p\}_{K_{\alpha_1}}} \sum_{q \in \{q\}_{K_{\alpha_1}}} \langle 1s, k_\gamma | \hat{O}_{\text{rad}} | p \rangle \rho_{pq}(t) \langle q | \hat{O}^+_{\text{rad}} | 1s, k_\gamma \rangle.$$

2.2. Observables from coincident measurements

The concept of irreversible change of quantum system internal properties in contact with a detector is one of the fundamentals in quantum theory of measurements. In our case, detection of L-REC or K$_{\alpha_1}$ photon at some moment $t_1$ breaks the process of evolution of the ion density matrix $\rho_{pq}(t)$ described by kinetic equation (2) with initial condition $\rho_{pq}(0) = \delta_{p0}\delta_{q0}$ and transforms this density matrix immediately into a new one corresponding to registration conditions of the performed measurement. After $t = t_1$ the evolution continues according to the same system of kinetic equations (2) starting from this new initial condition.

2.3. Distribution over the entrance parameter $x_0$

To bring calculations described above to real observables, all characteristics of the process under consideration, such as (3) and (4), must be convoluted with distribution of the well-channeled fraction of the beam over the ion entrance parameter $x_0$. At the moment, general understanding of this distribution remains not detailed enough. In our case, qualitatively, dechanneling and multiple scattering of the propagating ion from target electrons as well as mechanical electron capture (MEC) processes damp the radiative capture effects as the ion approaches close to
channel walls. Our preliminary calculations show, in agreement with recent experimental works in the field, that dominating role of radiative electron capture in forming X-ray spectra of channeled ions is limited by rather narrow (not exceeding a channel half-width) zone near the central plane of the channel. Taking into account successful application of this concept in our earlier studies [3, 4] on the RCE (the Okorokov effect), we introduce the width $x_0^{\text{max}}$ of the well-channeling zone as a free parameter into REC calculations as well.

3. Calculations
Numerical simulations in this work are performed for 20 MeV/u Ar and 60 MeV/u Kr nuclei incident on (220) planar channel of Si crystal 10 $\mu$m in thickness. A photon detector placed in a specific direction can measure differential (with respect to the direction) yield of L-REC and K$\alpha$ photons normalized for one incident nucleus. Registration of X-ray photons in coincidence with H-like ions at the exit of the target gives the spectrum corresponding to well-channeled ions. Fig. 1 represents the example of such a spectrum in the case of incident 20 MeV/u Ar$^{18+}$. Calculations without the mixing of $[n = 2]$ ionic states show its important role in the spectrum.
Examples of angular distributions (normalized to 1) of $K_{\alpha 1}$ photon yield in coincidence with L-REC photon registered in specific direction are shown in Fig. 2 and Fig. 3 for argon and krypton cases correspondingly. In channeling conditions angular correlation between L-REC and $K_{\alpha 1}$ photons is considerably lower compared to the case of free ion. In the case of planar channeling the angular correlations observed in channel plane and in the plane perpendicular to it differ due to the axial symmetry breakdown.

4. Conclusions
Calculation results indicate the significant role of the Stark mixing of $|n = 2|$ ionic states in formation of the X-ray spectra including L-REC line and $K_{\alpha}$ lines arising after REC event. Angular correlation between L-REC and $K_{\alpha 1}$ photons in channeling condition differs considerably in comparison with the case of a free ion. The results obtained in the cases of 20 MeV/u $Ar^{17+}$ and 60 MeV/u $Kr^{35+}$ ions show qualitatively similar features. This shows the importance of the Stark mixing consideration in REC studies in a wide range of ion energies and masses.

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