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SHARING OF THE ALIGNMENT IN DOUBLY IONIZED HEAVY ATOMS

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Abstract: Angular distribution of L₃ x-ray lines was calculated for doubly ionised atoms (L₃, M) in the framework of semiclassical approximation. Hydrogen-like wavefunctions, straight line projectile path and independent electron picture were assumed for the description of the ionisation process. From the calculation it was concluded, that the alignment transfer and the dealignment modifies significantly the L₃ subshell alignment.

In the last years the L₃-subshell alignment studies in heavy element were extended for heavy projectiles ([1], [2]). In these measurements the diagram and satellite lines were not resolved, and the obtained anisotropy parameters of the x-ray transitions characterise the alignment of the multiply ionised atoms. In the multiply ionised atoms before the x-ray transitions different processes may take place, which share on the alignment. The Auger and Coster-Kronig processes can carry out part of the anisotropy of the ionised atomic ensemble, and they can modify the vacancy distributions. The holes interact through the Coulomb field, and (as in the perturbed angular correlation) the alignment can be transferred between the different subshells. This interaction is large between the L₃ and M subshells, while it is small between the L₃ and N subshells (the only exception is the N₃ subshell). To get better understanding of this processes, as a first step, we studied the alignment of the doubly ionised atoms.

To see the importance of the double ionisation, at first the double ionisation cross sections were calculated in the following way: the ionisation probabilities as functions of the impact parameter were calculated in the semiclassical approximation (SCA) [3] for the L and M subshells, and the product of them for the L₃ and the different M-s were integrated over the impact parameter. Here and in the followings straight line projectile path was used in the SCA calculations, and the validity of the independent electron picture was assumed. In this calculation the (1-1/n)ⁿ⁻¹ type factors (where n is the number of the electrons on the regarded subshell) were neglected.
(Papp et al. 1987, to be published in J. Phys. B.: At. Mol. Phys.). The ratio of the double ionisation cross sections to the L$_3$ subshell ionisation cross section are proportional to $Z_i$ ($Z_i$ denotes the atomic number of the projectile). As a typical example, the results of our calculation are shown in fig. 1 for uranium target. The double ionisation cross section can reach relatively large value with increasing $Z_i$.

![Graph showing double L$_3$Mi (i=1,2,...,5) to single L$_3$-subshell ionisation cross section ratios for uranium bombarded by light ions as a function of the bombarding energy: \ldots\ldots\ldots M_1,\ldots\ldots\ldots M_2,\ldots\ldots\ldots M_3,\ldots\ldots\ldots M_4,\ldots\ldots\ldots M_5,\ldots\ldots\ldots M_6.]

Figure 1. Double L$_3$Mi (i=1,2,...,5) to single L$_3$-subshell ionisation cross section ratios for uranium bombarded by light ions as a function of the bombarding energy: \ldots\ldots\ldots M_1,\ldots\ldots\ldots M_2,\ldots\ldots\ldots M_3,\ldots\ldots\ldots M_4,\ldots\ldots\ldots M_5,\ldots\ldots\ldots M_6. total M.

Since the fine structure interaction energies [6] between the L$_3$ and M subshell holes are comparable with the widths of the double ionised states [5,6], this interaction can modify the alignment of the L$_3$ subshell and the angular distribution of the L$_3$ x-ray lines. The angular distribution of the L$_3$ x-ray lines of doubly ionised atoms with an aligned M vacancy can be described by the well-known perturbed angular correlation method [7]. In this method the ionised atomic ensemble is characterised by the density matrix. In the independent electron picture the elements of the density matrices of doubly ionised atoms are the products of the scattering amplitudes of the two holes. In the present work the scattering amplitudes were calculated for the L$_3$ and M subshell as a function of the impact parameter in SCA, and the density matrix elements created from the amplitudes were integrated over the impact parameter. For calculation of the angular distribution we used the fine structure energy splitting value of Parente at al [4].

The L$_3$ x-ray angular distribution of singly and doubly ionised atomic ensemble can be written as

$$W(\Theta) = W_0 \left(1 + \beta \mathcal{P}_2(\cos(\Theta))\right),$$

where the $\beta$ anisotropy parameter is

$$\beta = \alpha \left(A_2(1) - 1\right) + \beta A_2(2).$$
Here I denotes the ratio of the double ionisation cross section to the $L_3$ subshell ionisation. $A^{(1)}$ and $A^{(2)}$ are the $L_3$-subshell alignment parameter of the singly and doubly ionised atoms. The $A_2$ alignment parameter characterises the atomic ensemble before the x-ray transition, and contains the effect of the interaction between the holes, and it is not determined completely by the ionisation processes. For the super Coster-Kronig transition probabilities in the $N$-shell we used the value of reference [6], and assumed that these transitions do not depend on the magnetic quantum number of the holes.

Figure 2. Light ion induced anisotropy parameter ($\beta$) of Au. Curves show SCA results for $N$ impact, assuming: --- single, single and double ionization. Experimental data of Jitschin et al. (1983):

- O impact, C impact.

There exist experimental data only for C and O ion impact on gold [1] in broad range of impact energy. For this reason we present the result of our calculation for N ion impact on gold, since the calculated alignment parameter has only small differences when $Z_1$ is changed by one. Our calculation shows (fig. 2), that the anisotropy parameter of the emitted x-rays of the singly and doubly ionised atoms differs significantly from the singly ionised one, and the angular distribution of the satellite lines are quite different from the diagram line. It can be seen from fig. 2, that the second hole produces not only realignment, but it produces alignment transfer too. This calculation shows the importance of the double ionisation in the $L_3$ subshell alignment studies. We remark that the validity of our results is limited by the used simple wavefunctions. Using more refined wavefunctions, and performing calculations with inclusion of higher-order terms of the Born series [6], theoretical data in better agreement with the experimental ones can be obtained.

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References.


