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ATOMIC K-SHELL DOUBLE HOLE CREATION DUE TO ELECTRON CAPTURE AND PHOTOIONIZATION

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Double core hole (DCH) states could be created in two different mechanisms. The first is core subshell electron capture by the nucleus and subsequent shake-process of an electron from the same subshell either to the high unoccupied state (shake-up) or to the continuum (shake-off) mostly due to instant changing of the nucleus charge by unity. Another way is photoionization, when one electron is "knocked out" from the subshell and the residual one undergoes shake-process resulting from changing in screened potential. Physics of the DCH currently attracts interest stimulated by new possibilities of their creation by X-ray free electron lasers and advanced synchrotron sources. Furthermore, DCHs might become a new tool for chemical analysis [1] and plasma diagnostics [2].

In this theoretical contribution we compare the two mechanisms of producing the DCH: K-electron capture and K-shell photoionization. General theoretical approaches to both problems are known, but we are not aware of such a comparison based on up-to-date models for many-electron atoms. We focus on DCH states in K-shell of ^{7}Be and ^{37}Ar (isotopes with natural electron capture radioactivity). The goal is to determine double K-vacancy production probability in both described channels. Also, we analyze shake-off electron spectra and compare the results with different theoretical approaches and experiment.

Our model is based on sudden approximation with the use of fully non-orthogonal sets of electron orbitals in initial and final states, accounting for j-splitting of the subshells. Expansions for transition matrix elements are obtained with ZAP_NO package [3]. Radial wave functions are constructed within the multiconfigurational Hartree-Fock method [4]. Photoionization calculations are performed with the use of B-spline R-matrix (BSR) software complex [5].

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The speaker is a student or young scientist

Yes

Section

1. Synchrotron and neutron radiation sources and their use in scientific and applied fields

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