MULTICONFIGURATION DIRAC-FOCK SIMULATION OF RESONANT AUGER DECAY OF 3d $\rightarrow$ 4p EXCITED Br

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The aim of this study is to identify and interpret the lines observed in the Auger electron spectrum following the $3d^{-1}4s^24p^6$ excitation in atomic Br*. Interpretation is done with the aid of multiconfiguration Dirac-Fock (MCDF) calculations.

The Br* $3d^{-1}4s^24p^6$ state was created by ultra-fast dissociation of HBr molecule upon $3d \rightarrow \sigma*$ excitation [1]. The resulting Auger decay spectra was measured at the soft X-ray beamline BL6U at Ultraviolet Synchrotron Orbital Radiation Facility (UVSOR) in Okazaki, Japan [2]. Monochromatized radiation from the beamline was introduced into a gas cell filled with the sample gas. Hemispherical electron energy analyzer (MBS-A1) was used to record the kinetic energies of the emitted electrons. The axis of the electrostatic lens of the analyzer was fixed at the magic angle (54.7°) relative to the direction of polarization of the incident synchrotron radiation.

In order to simulate the $3d$ hole decay, energies and wave functions of the excited, $3d$ hole and final ionic states of atomic Br were obtained from MCDF calculations, which were performed using the relativistic atomic structure code GRASP92 [3]. The subsequent Auger decay was treated as a two-step model and simulated using the AUGER component of the RATIP suite [4]. Convincing agreement with the measured spectra was reached when the final state of the first step of the Auger decay was generated and calculated including the configurations $4p^6$, $4s^14p^5$, $4s^14p^44d^1$ (these three have a possibility of further Auger decay), $4s^24p^4$, and $4s^24p^34d^1$. To simulate the second step of the decay a final state consisting of configurations $4s^14p^4$, $4s^24p^3$, and $4s^24p^24d^1$ was generated.

Configuration interaction between the configurations $4s^14p^5$ and $4s^24p^34d^1$ was found to be a prominent contributor causing the rich line structure seen in the spectra. The apparent absence of $4s^04p^6$ lines is explained by fast super Coster-Kronig decay to $4s^14p^4$ states, which broadens the respective lines into the background.

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