Towards understanding the Auger cascade following Xe $3d_{5/2}$ photoionisation

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Synopsis The Auger cascade following Xe $3d_{5/2}$ photoionisation has been simulated using a recently developed Monte Carlo model. Good agreement between the simulation and experiment has been achieved. This agreement allows informed speculations to be made about the origins of several structures observed in the measurement.

High-efficiency multi-electron coincidence measurements have been made possible since the introduction of a new magnetic bottle time-of-flight spectrometer by Eland *et al.* [1]. This allows detailed investigation of Auger-electron cascades following inner-shell ionisation by synchrotron radiation. Suzuki *et al.* [2] recently measured the energy correlation between the electrons emitted in the first step of the Auger cascade (280-600 eV) and the electrons (0-160 eV) released in the subsequent steps following Xe $3d_{5/2}$ photoionisation using a multi-electron coincidence technique (see Figure 3 in Ref. [2]). This measurement revealed several intriguing structures such as diagonal stripes and vertical bands spanning from 0 to 160 eV. The origin of the diagonal stripes is well established as the shake-off process accompanying Auger transitions [3], which is also called double-Auger decay. The double-Auger decay involves simultaneous emission of two electrons and they share the total available energy asymmetrically. However, the origin of the vertical bands is less well known and is usually neglected.

In this study, we simulate the Auger cascade following Xe $3d_{5/2}$ photoionisation at a photon energy of 924 eV (same as Ref. [2]) using a recently developed Monte Carlo model of atomic relaxation, `BrIccEmis` [4]. We calculated the shake-off probabilities for $3d_{5/2}$ ionisation and Auger transitions in the first step of the cascade based on the theory in Ref. [3]. The energies of Auger transitions in the second and following steps of the cascade, are usually too low for the sudden approximation used in Ref. [3] to be valid. Figure 1 shows the simulated energy-correlation spectrum resulting from the Xe $3d_{5/2}$ photoionisation. The diagonal stripes at the available energies of 415 and 490 eV observed in Ref. [2] are reproduced in the simulation although the calculated total energy for the former stripe is slightly lower than the measurement. The vertical bands are also reproduced and the intensity of these bands increases near the top edge (∼160 eV) which agrees well with the experiment. According to the simulation, these bands are created by the shake-off process accompanying the photoelectrons, which means they are formed by the same mechanism as the double-Auger decay.

Here we will discuss the formations of the double-Auger stripes and the shake-photoelectron bands in detail as well as the implications of this theoretical investigation on future studies of the Auger cascade.

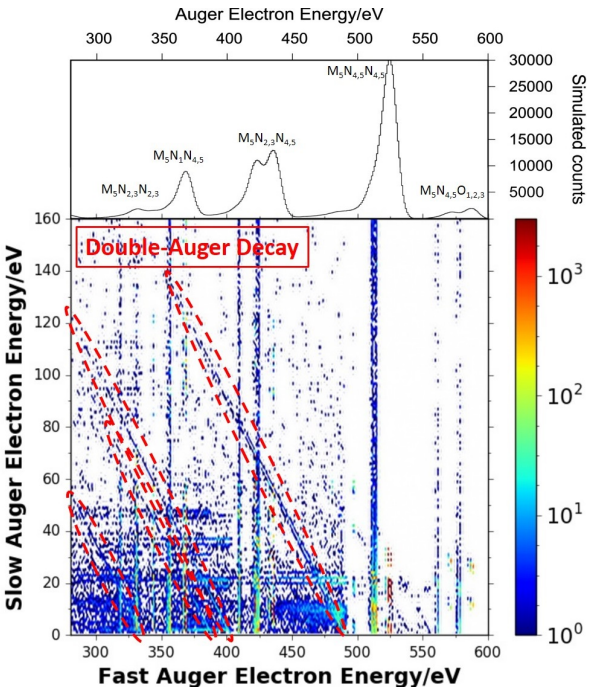

Figure 1. Simulated energy-correlation spectrum between fast Auger electrons (280-600 eV) and slow Auger electrons (0-160 eV) emitted following Xe $3d_{5/2}$ photoionisation. The upper panel shows the non-coincident spectrum, which is folded with an an approximate lineshape, for electron energies of 280-600 eV. The energy-correlation spectrum is unfolded and binned with 1 eV bin size in both x and y axes.

References

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