ESRF	**Experiment title:** Core-hole recombination in the 5*d* transition metals Hf and Ta using resonant Auger emission spectroscopy	**Experiment number**: HE-2567
Beamline: ID16	**Date of experiment**: from: 16/7/2008 (08:00) to: 22/7/2008 (08:00)	**Date of report**: 13/08/2008
Shifts: 18	**Local contact(s)**: Laura Simonelli	*Received at ESRF:*

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Report:

We have investigated for the first time the core-hole recombination processes in the 5*d* transition metal tantalum using Resonant Auger emission spectroscopy at high photon energies. We have observed the resonant Raman to normal Auger transition in the $L_3M_{4,5}M_{4,5}$ non-radiative (Auger) decay channel while tuning the photon energy through the 2*p*-5*d* absorption edge.

A particularly important part of the fundamental physics underlying resonant spectroscopies is the core-hole recombination which results in the emission of the photon or electron to be detected. For an excitation in the vicinity of an absorption edge it is well established that the two-step model often employed for Auger or x-ray emission often fails. Instead the creation and subsequent decay of the core hole must be treated in a one-step formalism [1]. In this resonant Raman regime the energy of the emitted electron or photon follows the incident photon energy, as opposed to the usual, off-resonant case where the emitted electrons or photons appear at a constant kinetic energy. The distinction between the two scenarios depends on the time needed for the excited electron to delocalise or lose energy in relation to the core hole lifetime [2].

A Ta foil was scraped in vacuum after an initial *ex situ* acid cleaning treatment. Photoemission spectra were measured on the VOLPE instrument mounted on ID16. With the high kinetic energies of the emitted electrons this technique becomes much more bulk sensitive, easing greatly surface cleanliness concerns. The Ta 2*p*-5*d* absorption edge was measured in fluorescence mode (see Figure 1a). The $L_3M_{4,5}M_{4,5}$ Auger spectra were then measured at various photon energies through this edge. The photon energies used are shown in Figure 1a and the resultant normalized spectra in Figure 1b. What is immediately clear from the data is that before the strong white line of the absorption edge the Auger spectra follow a resonant Raman behaviour, that is they are emitted at constant binding energies. After the peak however they are emitted at constant kinetic energies i.e. the normal Auger regime. There is also an evident resonant enhancement of the Auger intensity moving through the edge. We are now beginning a complete analysis of these spectra based on the calculated multiplets of the $M_{4,5}M_{4,5}$ two hole final state convoluted with the calculated partial density of empty *d* states [3].

The primary aim of this proposal is to compare the resonant behaviour of emissions from Augers originating from different core levels (see original proposals). In this case the $L_3M_{4,5}M_{4,5}$ spectra are to be compared with the $L_3N_{4,5}N_{4,5}$ and $L_3O_{4,5}O_{4,5}$ spectra. Although these latter two lie in the reported 6 – 10 keV range of the

VOLPE spectrometer [4], (they are located between 9 keV and the Ta edge at 9.881 keV), in practice the VOLPE spectrometer is limited to 9 keV [5]. Thus we were unable to perform this essential part of the study. We intend to apply for further beamtime to complete this work at ID32 which has a spectrometer (Phoibos 225 from SPECS) which easily reaches the required energies.

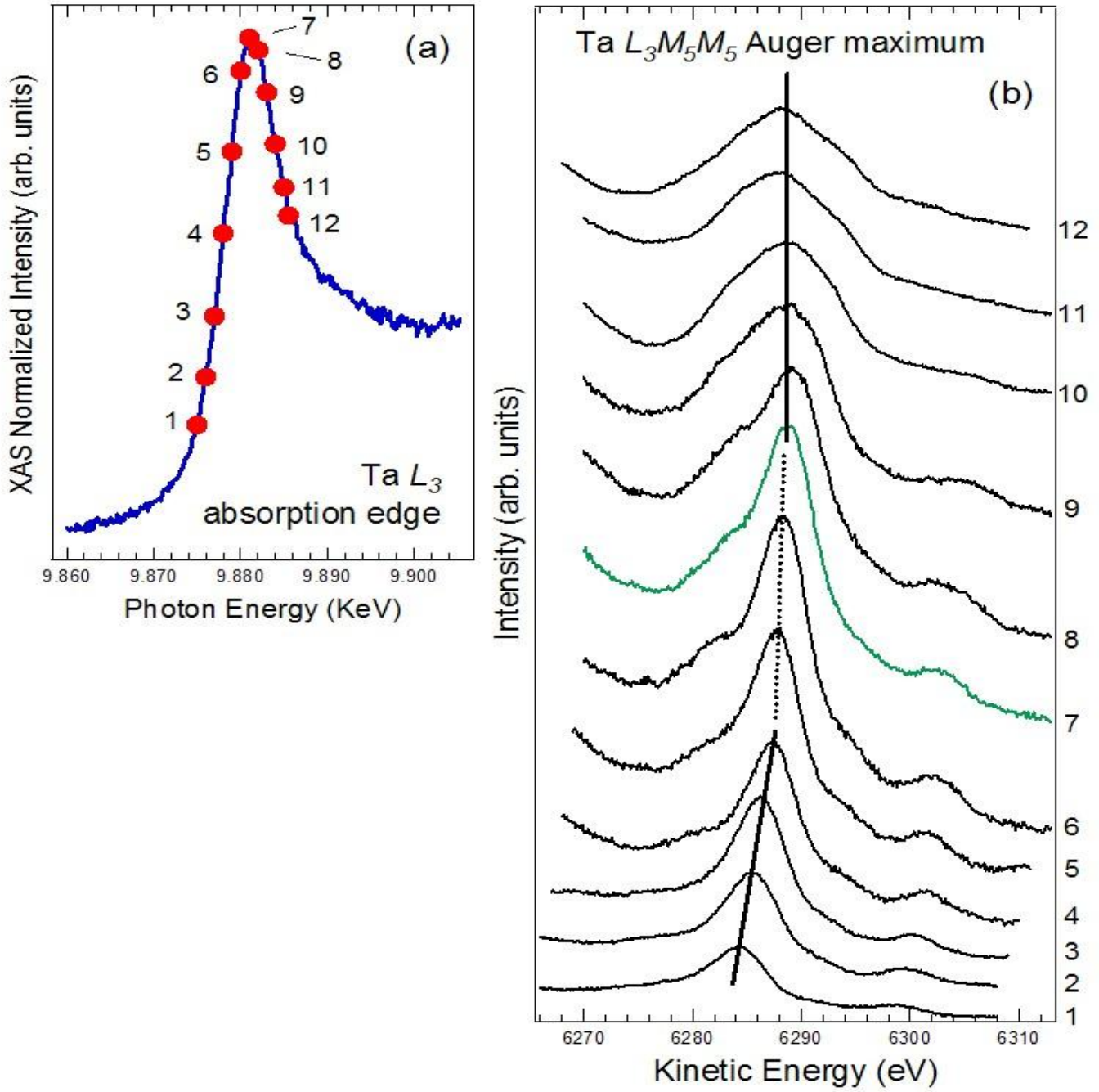

Figure 1: Resonant Auger electron spectroscopy following the *Ta* $L_3M_{4,5}M_{4,5}$ channel through the 2*p*-5*d* absorption edge. The transition from resonant Raman (constant binding energy) to Auger (constant kinetic energy) is clearly visible.

References:

1. T. Åberg and B. Crasemann, in *Resonant Anomalous X-ray Scattering*, eds. G. Materlik, C.J. Sparks and K. Fischer (Elsevier, Amsterdam, 1994) p. 431
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3. W. Drube *et al.*, *Phys. Rev. Lett.*, **74** (1995) 42
4. P. Torelli *et al.*, Rev. Sci. Instr. **76**, 023909 (2005)
5. G. Panaccione, *private communication*