X-ray hypersatellite spectra of hollow atoms

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Introduction

- A K-hollow atom is an ion which has a **totally empty** K **shell**, while its outer shells are occupied.

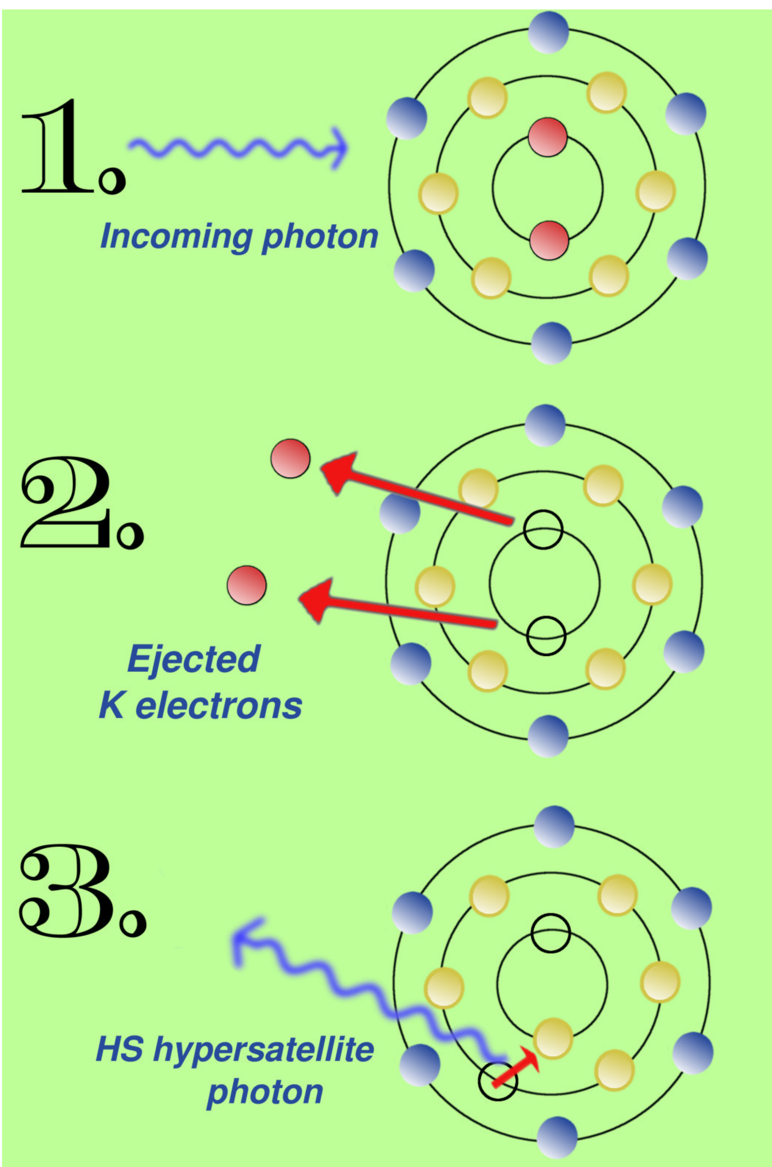

Figure 1: The formation mechanism of a hollow atom and the creation of a hypersatellite ¤uorescence photon.

- The radiative relaxation of such an atom yields the so-called **hypersatellite** (HS) spectra.
- Such spectra are denoted e.g. $K^h\alpha_{1,2}$ and $K^h\beta_{1,3}$, which originate in the K-hole spectator transitions $1s^{-2} \rightarrow 1s^{-1}2p^{-1}$ and $1s^{-2} \rightarrow 1s^{-1}3p^{-1}$, respectively.

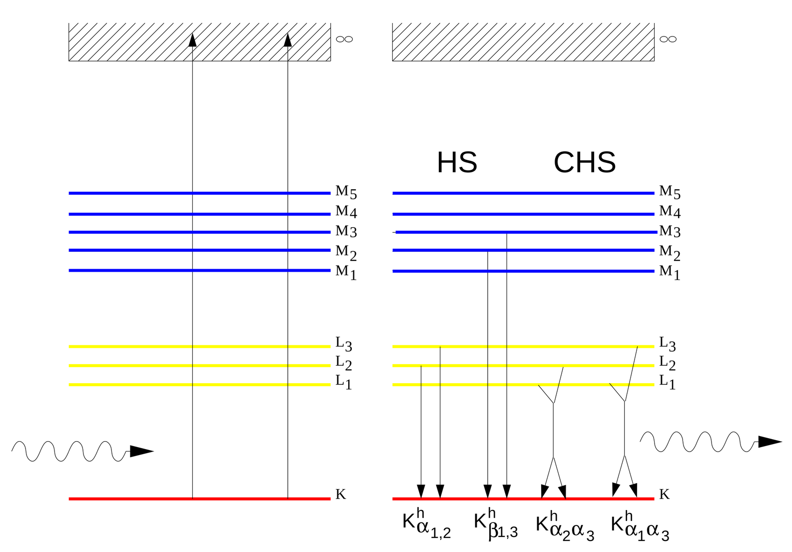

Figure 2: The transitions involved in the production of the hypersatellites (HS) and correlated hypersatellites (CHS).

- Hypersatellites allow the study of *intrashell correlation*, *Breit interaction*, *QED effects in atoms* and *relativity*
- The $K^h\alpha_1$ hypersatellite line originates in a spin-¤ip transition, which is forbidden in the LS coupling scheme but fully allowed in jj coupling $\Rightarrow$ the spectra are **highly sensitive to the coupling scheme in the atom**.
- Single-photon absorption results in an excitation of two electrons which is possible only because, and hence allows the study of **intra-shell correlation**.

Methodology

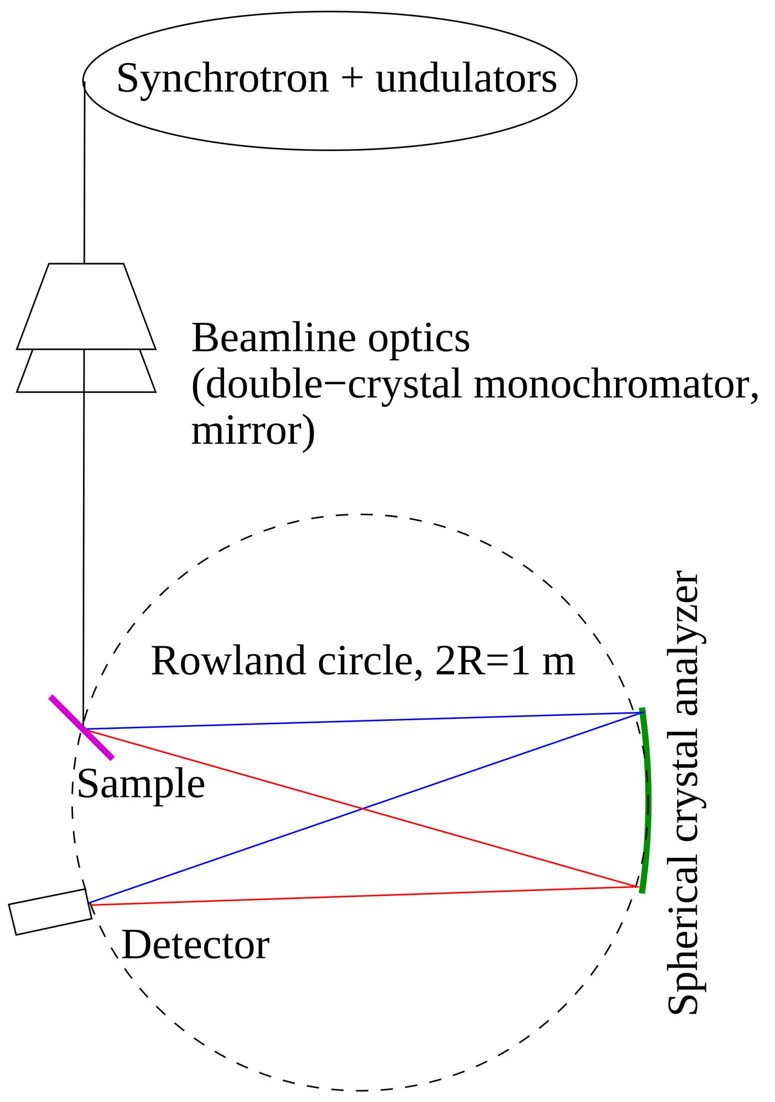

Figure 3: Experimental setup. High resolution is achived by using Bragg angles $\sim 90°$ in the spectrometer.

Figure 4: Upper panel: the European Synchrotron Radiation Facility in Grenoble, France. Lower panel: the National Synchrotron Light Source in Brookhaven National Laboratory, New York, USA.

- The best way to produce hollow atoms in a clean and controlled way is photoionization by **monochromatic synchrotron radiation** [*Fig. 3*]
- The hypersatellite ¤uorescence photons are detected using a **scanning-crystal spectrometer** [*Fig. 3*]
- The experiments have been performed at the European Synchrotron Radiation Facility (ESRF, France) beamlines ID16 and ID15B, and at the National Synchrotron Light Source (NSLS, USA) beamline X25. [*Fig. 4*]
- **Experiments are very challenging**: the cross-section for the production of hypersatellite lines is of the order of 10^{-4} of that of the corresponding diagram lines.

Results

- The experimental hypersatellite spectra are compared to results of *ab-initio* calculations done with the relativistic multi-con£gurational Dirac-Fock (RMCDF) code `GRASP`.
- The Cu $K^h\alpha_{1,2}$ hypersatellite lines show clearly how **the** LS**-forbidden** $K^h\alpha_1$ **line is much weaker than the allowed** $K^h\alpha_2$.

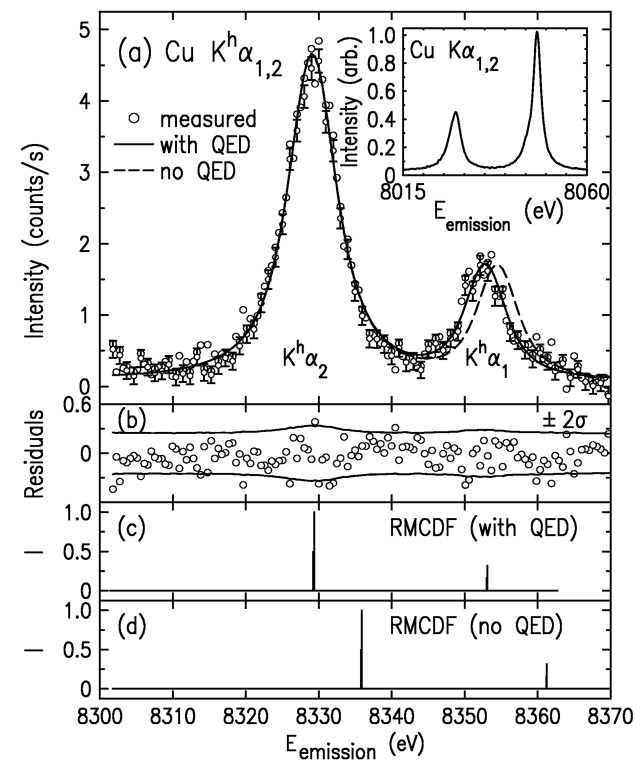

Figure 5: The Cu $K^h\alpha_{1,2}$ hypersatellite emission lines. The inset shows the $K\alpha_{1,2}$ diagram spectrum. Note the reversed intensity ratio.

- The variation of the $K^h\alpha_{1,2}$ line's intensity ratio as a function of Z reveals **how the dominating coupling scheme evolves gradually from** LS **toward** jj with increasing Z.

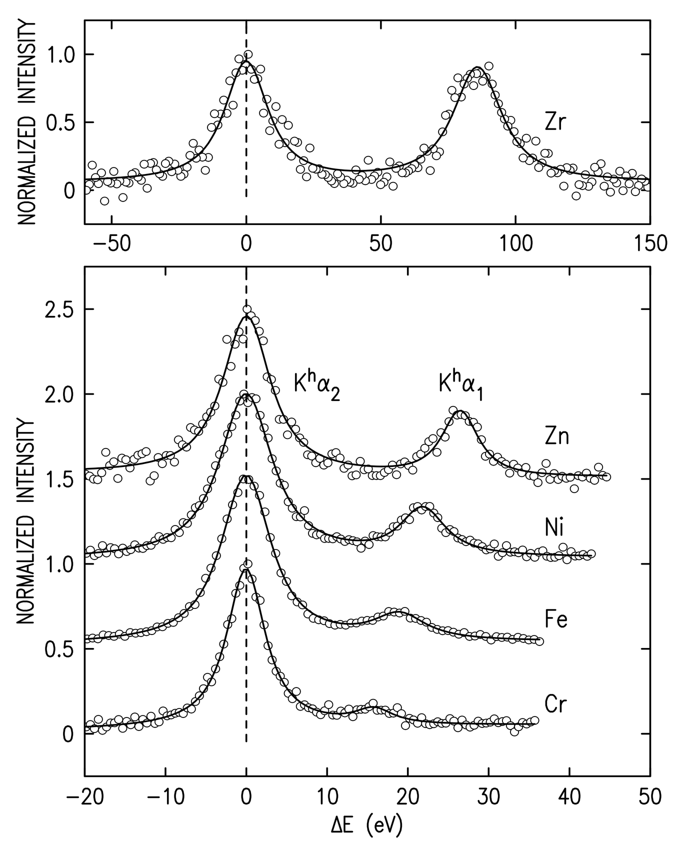

Figure 6: The $K^h\alpha_{1,2}$ hypersatellite spectra of various elements.

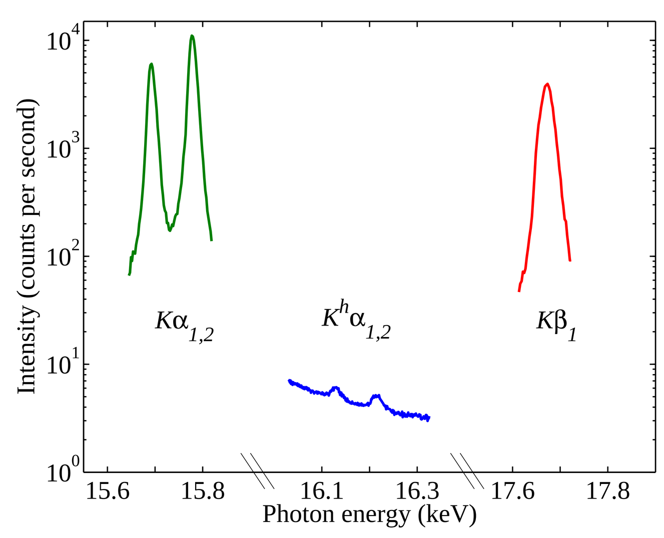

Figure 7: The diagram $K\alpha_{1,2}$ and $K\beta_1$ and the hypersatellite $K^h\alpha_{1,2}$ lines of Zr measured at the ESRF beamline ID15B.

- The $K^h\beta$ lines are even weaker than the $K^h\alpha$ spectra. However, their measurement yields important information on the energies of the outer shells of the hollow atom. [*Fig. 8*]

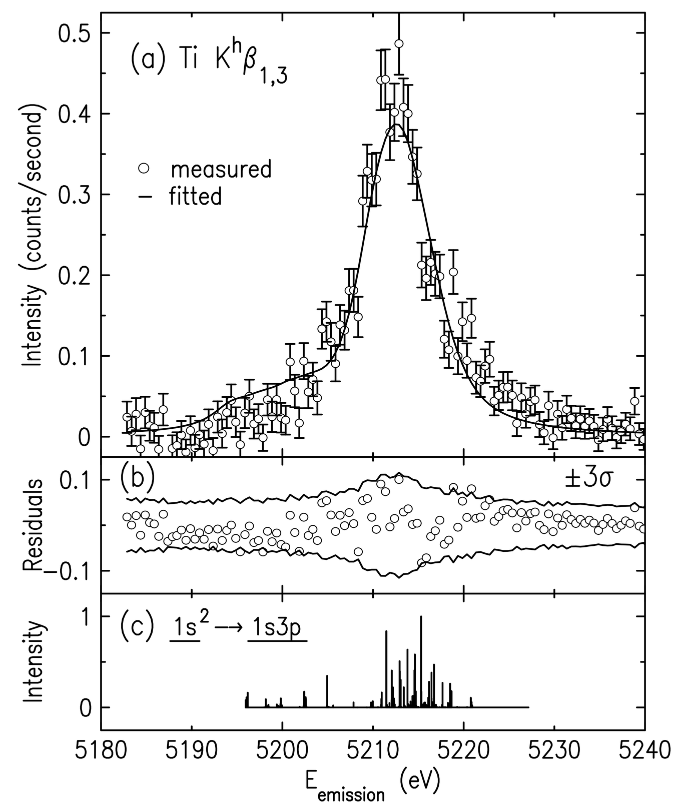

Figure 8: The measured Ti $K^h\beta$ HS spectrum (circles) compared to *ab-initio* RMCDF calculations (solid line).

- The evolution of the hypersatellite lines' intensity as a function of the exciting-photon energy [*Fig. 9*] shows **a very large saturation range**, not explained by any theoretical model to date. Theoretical calculations in the near-threshold region are clearly needed!
- The continuous rise in intensity from threshold suggests a **pure shake-off character** for the production of the second K hole.

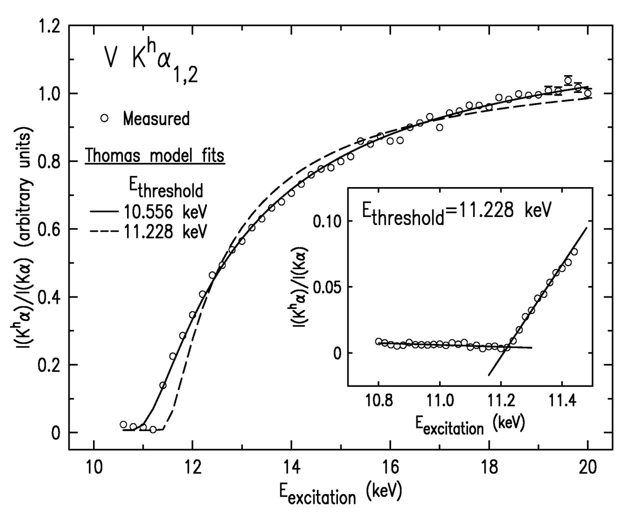

Figure 9: The intensity evolution of the V $K^h\alpha_{1,2}$ hypersatellite lines.

Publications

1. R. Diamant, S. Huotari, K. Hämäläinen, C.-C. Kao, and M. Deutsch: *Cu* $K^h\alpha_{1,2}$ *hypersatellites: Supratreshold evolution of a hollow-atom x-ray spectrum*, Physical Review A 62, 052519 (2000).
2. R. Diamant, S. Huotari, K. Hämäläinen, C.-C. Kao, and M. Deutsch: *Evolution from threshold of a hollow atom's x-ray emission spectrum: The Cu* $K^h\alpha1,2$ *hypersatellites*, Physical Review Letters 84, p. 3278 (2000).
3. R. Diamant, S. Huotari, K. Hämäläinen, R. Sharon, C.-C. Kao, and M. Deutsch: *The diagram x-ray emission spectra of a hollow atom: The* $K^h\alpha_{1,2}$ *and* $K^h\beta_{1,3}$ *hypersatellites of Fe*, Physical Review Letters 91, 193001 (2003).