

# Near-edge anomalous Rayleigh scattering in Cu ions

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## 1. Introduction

Elastic scattering cross-sections for free atoms at energies far from atomic orbital edges are measurable to high accuracy, surpassing that of photo-absorption (Sparks and Ice, 1997). While computationally intensive S-matrix calculations have been confirmed experimentally for a wide range of angles and energies (Bradley et al., 1999), near to core electron ionisation thresholds, where anomalous scattering terms dominate, data are of poorer quality. New techniques are sought to complete measurement sets and test hybrid methods of calculating cross-sections that utilise S-matrix corrections for angular-dependent components of the anomalous scattering terms.

Over the last 2 years, direct measurement of anomalous scatter cross-sections have been attempted at synchrotron beamlines (Hugtenburg et al., 2002; Hugtenburg and Bradley, 2003) utilising dilute solutions of salt solutions and thin films of the associated neutral metal. These results confirm predictions from the independent particle approximation (IPA), in particular the oscillatory nature of below edge structure due to bound-bound (b–b) resonant intermediates and increases in the size of b–b resonances with decreasing  $Z$  (Carney et al., 2000) underlining potential application to the study of the low- $Z$  electrolytes in biological systems.

In order to achieve high precision in the determination of cross-sections, we investigate a modification of a technique used for measurements of elastic scatter cross-sections in gases where the cross-section of a

known gas is used to calibrate a second gas (Young et al., 2001). Elastic scatter in the medium must be well characterised and tabulations of form-factors for amorphous materials (e.g. Peplow and Verghese, 1998) provide a set of known cross-sections, which converge at high angles to IPA (Goncalves et al., 1994).

## 2. Experimental methodology

Beamline 16.3 at the Daresbury synchrotron source and beamline BM28 at the ESRF synchrotron (Grenoble) have been used in investigating three kinds of target: vapour-deposited metals on glass; doped sol–gel glasses, with charge states of +1 and +2 on the dopant metal ion; and aqueous metal ion solutions. Measurements of thin-film neutral Cu were made at the  $\langle 220 \rangle$  diffraction peak; momentum transfer was preserved with energy changes by varying the scatter angle (around  $55^\circ$ ). For the solutions and samples of glass, diffraction measurements were obtained over a wide range of angles. Solutions were contained in a thin ( $8\ \mu\text{m}$ ) kapton windowed cell.

Elastically scattered photons were measured using a HPGe detector (resolution less than  $0.5\ \text{keV}$  FWHM), being typically unresolved from the Compton scattered component and the emergent  $\text{K-}\beta$  fluorescence. The  $\text{K-}\alpha$  fluorescent component has been recorded, enabling characterisation of the  $\text{K-}\alpha$  component presuming energy independence of the ratio of the  $\text{K-}\alpha$  to  $\text{K-}\beta$  yield. The non-resonant Compton component was predicted from the relativistic impulse approximation. The targets were sufficiently thick for scatter contributions to be relatively insensitive to variations in sample

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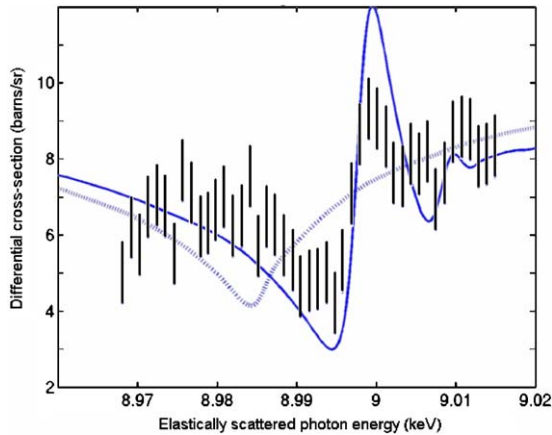


Fig. 1. Differential cross-section (Barns/sr) measured (points) and calculated (dark line) for 0.1 Mol/l solution of  $\text{Cu}^{2+}$  ions for  $90^\circ$  elastic scatter in the vicinity of the K-edge of copper (8.979 keV). The calculated data have been Lorentz broadened by 5 eV. Predictions for neutral copper are also given (light line).

thickness; multiple scatter was handled by Monte Carlo methods.

### 3. Results and discussion

A Slater exchange potential with a Latter tail corrected for the higher charge states (Kissel, 2000) was used to obtain absorption cross-sections and the chemical shift of the K-edge and b–b resonance oscillator strengths. While b–b resonant features are not clearly observed in the absorption spectra due to the close proximity of excitation channels and the ionization threshold, they are observed in the measured elastic scatter cross-section for aqueous  $\text{Cu}^{2+}$  ions (Fig. 1).

Calculated amplitudes broadened by 5 eV gave good agreement with theoretical data at both 0.01 and 0.1 Mol/l but greater distortions at 1 Mol/l suggesting an effective upper bound in ionic concentration to the application of IPA. Cross-sections in Cu metal are in relative accord with previously published data using indirect methods (e.g. Stanglmeier et al., 1992) though differing somewhat from the calculation for neutral Cu shown in Fig. 1. Our model does not include a strong 1s–4p shake-down resonance which occurs in some metals. Shakedown is not observed in the aqueous ions, further supporting the validity of IPA.

### 4. Conclusion

Our group has been examining the measurement of elastic scattering of atoms and ions imbedded in amorphous systems, including ions contained in aqueous solutions and sol–gel glasses, where the independent particle approximation may have reasonable validity. These systems offer the potential for measuring a wider range of atoms including metals in a range of ionic states that are observed for example in biological systems.

Measurements of near K-edge elastic scattering from the Cu atom and ions have been obtained in a variety of environments in an attempt to understand features in the intensity profile at the atomic level and to seek possible exploitation of atomic information including charge-state and valence structure in analysis.

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