# X-ray Extended-Range Technique for Precision Measurement of the Imaginary component of the X-Ray Atomic Form Factor for Copper (8.85 keV - 20 keV) using Synchrotron Radiation

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We introduce the X-ray Extended-Range Technique for accurate measurements of the mass attenuation coefficient and the imaginary component of the atomic form factor. We present results of this technique for copper in the range from 8.85keV to 20keV, with accuracies of $0.3\% - 0.5\%$. This represents a major development compared to the current best accuracies of order 10% using atomic vapours [1], and compared to the discrepancies between earlier experimental techniques of order 10% [2]. Accurate evaluation of these coefficients are potentially invaluable for applications to structural evaluation using crystallography, XAFS, DAFS and MAD techniques, and are currently beyond the quoted accuracies of theoretical calculations. An illustration of detailed XAFS recovered by this technique is given in Fig. 1, showing not just the relative structure but also the absolute calibration of the result.

The reported accuracies exceed those of available theories [3,4] and therefore the results allow tests of underlying assumptions in theoretical work including the independent particle and isolated atom approximations, computational difficulties, solid state and nearest neighbour effects, and especially alternative relativistic approaches. Dirac Hartree-Fock, Hartree-Slater, relativistic multipole and all-orders calculations can then be compared.

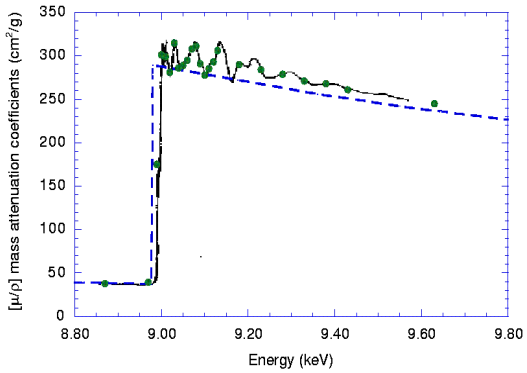


Figure 1: Detailed XAFS (X-ray Anomalous Fine Structure) measurement of the Cu K-edge on an absolute scale, compared to theory (– – –, Chantler, 1995,[4]). ● this work (dot size represents $10\sigma$). The relative observations [6] ( — ) are in excellent agreement. Theory is inadequate near absorption edges due to the independent particle and isolated atom approximations used.

While the accuracy is high, the method achieves a still higher precision, and indicates reproducibility approaching 0.02% [Fig. 2]. This reproducibility suggests that future experiments may be able to yield accuracies approaching this figure, which would open up a large range of critical tests of radial electron density wavefunctions and MCDF / S-matrix computational approaches [5].

This paper summarises key developments of this new technique. Current theoretical and experimental discrepancies of order 10% can now be addressed. In particular, the investigations of solid state structure and near-edge atomic physics become much more insightful.

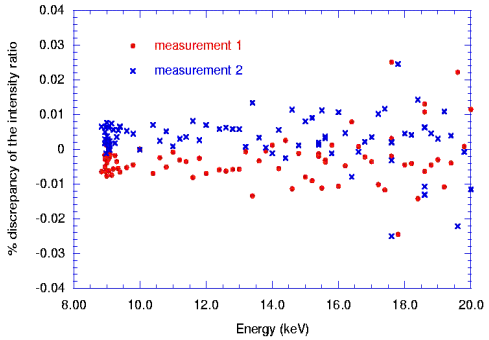


Figure 2: Demonstration across large ranges of energy of extremely high intrinsic precision from two independent sets of data. The 0.01% - 0.02% residual difference between the results of the two sets is a systematic and not a random effect, so the statistical uncertainty from the data is smaller than this.


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[6] Wong, J., 'Reference X-ray Spectra of Metal Foils', EXAFS materials, Inc., 871 El Cerro Blvd, Danville CA USA (1999). These excellent results have a very fine grid giving the local structure with greater detail than most published results, but have relatively poor statistics and low accuracy. Hence the data is excellent for testing structural reproducibility of XAFS but the values must be scaled and adjusted to give an absolute result as represented in the figure.