

June 4

New Theoretical Investigation Resolving Discrepancies of Atomic Form Factors and Attenuation Coefficients in the Near-edge Soft X-ray Regime

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Abstract

Reliable knowledge of the complex X-ray form factor and the photoelectric attenuation coefficient is required for crystallography, medical diagnosis, radiation safety and XAFS studies. Discrepancies between currently used theoretical approaches of 200% exist for numerous elements for X-ray energies from 1 keV to 3 keV. This work addresses key discrepancies and derives theoretical results in near-edge soft X-ray regions.

DHF wavefunctions are employed and computational and convergence issues are of direct concern. Comparisons with simpler wavefunctions including additional relativistic corrections to the form factors are insightful.

The current result improves upon the theoretical uncertainty in these regions to an estimated standard deviation of 20% - 30% .

Keywords: Attenuation Coefficients, Soft X-rays, Atomic Form Factors

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A new tabulation is reported (Chantler, 2000) which computes atomic form factors and attenuation coefficients for elements with absorption edges in the soft X-ray regime, 1 - 3 keV. This improves significantly upon earlier work (Chantler, 1995) in this regime, and complements the earlier work in other energies.

The primary improvement of this computation is to continue to use DHF wavefunctions but to improve the wavefunction and computational convergence, particularly for L_{II} , L_{III} , M_{IV} and M_V edges where they were significantly affected by the consequences of minor imprecision in K , L_I and M_I orbital wavefunctions. This new result arose in response to large discrepancies observed between three theoretical tabulations commonly used as databases for attenuation and photoelectric absorption coefficients (Chantler, 1995; Saloman and Hubbell, 1986; Saloman, Hubbell and Scofield, 1988; Henke et al., 1993). All of these databases have this convergence or smoothing problem in these regions, because of the difficulty of correlation between orbital wavefunctions in the medium-Z neutral atoms.

The new tabulation (Chantler, 2000) should be used with the earlier work (Chantler, 1995) to provide f_1 and f_2 form factors and $[\mu/\rho]_{PE}$ for all elements up to $Z=92$ from 0.01 keV to 1000 keV.

For convenience of users in the field, a fine grid is provided for the regions of direct interest in the new computation, and a coarse grid for $Z=30-36$, $Z=60-89$ from 0.1 keV to 10 keV; this follows the Grodstein grid energies used in earlier tabulations and by other researchers.

The energy range covered exceeds that for normal X-ray diffraction and crystallography studies but allows limitations and specialised experiments to be investigated with reference to updated and corrected theory. Solid target effects, correlation, nuclear resonances and uncertainties should be noted carefully in applications below 1 keV or above 100 keV.

Linear attenuation coefficients, scattering cross-sections, structure factors and scattering coefficients may be derived simply from the tabulated data, and may also make use of scattering coefficients contained in Hubbell and Overbo (1979) (σ_{coh}), and Hubbell et al. (1975) (σ_{incoh}), or in recent work of Pratt (2000), particularly for high-energy contributions

or for comparison of scattering cross-sections.

Applications of these results include crystallography, electron density studies, X-ray Anomalous Fine Structure experiments, attenuation and absorption calculations for medical and radiation exposure and, for example, the sensitivity of mammographic filtered exposures to simulated ghosts, or the efficacy of radiation shielding.

The accuracy of f_2 and μ or $[\mu/\rho]_{PE}$ in (Chantler, 2000) and (Chantler, 1995) in a central X-ray region well away from edges is estimated as 1%. Chantler (1995) yielded maximum errors of 68% and 78% in the regions covered by the new work, with an estimated standard deviation in these regions of 50%. In these and similar cases the Scofield result yields 80% and 220% errors near the edge (or 4-5 σ errors); The estimated uncertainty in the new work (for energies and edges above 1 keV) is 20-30% compared to a monatomic gas form factor (ignoring the effects of solid state structure and XAFS), representing an improvement of a factor of 3-4.

An interesting comparison is given by results of measurements of the noble gas Kr, $Z=36$ (Fig.1). The structures of Chantler (1995), Henke et al. (1993) and Scofield (1973) are in error, particularly for the L_{III} edge region. Conversely, Chantler (2000) agrees with all experimental structure for the full energy range. The precision of the experimental data set is quite high, possibly approaching the 1% level.

We would like to thank J. H. Hubbell and E. Saloman for their helpful interactions and promptings towards this research; and also to P. J. Mohr and J.-L. Staudenmann at NIST, and D. C. Creagh for their comments, support and encouragement.

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FIGURES

FIG. 1. Plot illustrating the consistency of near-edge structure between experiment (Wuilleumier, 1972) and that predicted by the new theoretical work, as opposed to earlier theory. $\text{Im}(f) = f_2$. The experimental values include contributions from scattering. $[\mu/\rho]$ (in cm^2/g) = f_2 (e/atom) $\times 5.02152 \times 10^5$.

Kr Z=36

