NEW MEASUREMENTS OF X-RAY FUNDAMENTAL PARAMETERS

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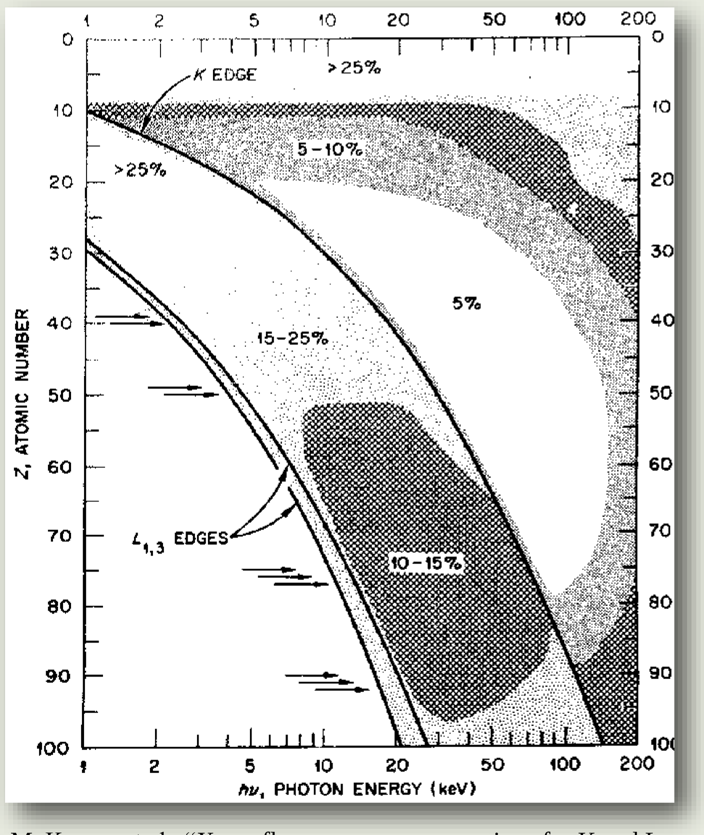
STATE OF THE ART

X-ray fundamental parameters are of the utmost importance for quantitative and qualitative X-ray based techniques. In reference-free methods, the quality of the analysis result is directly dependent on the reliability of such parameters characterizing the interaction between X-ray photons and matter: μ, ω, f. New values of these parameters can be obtained either by experimental work, using modern facilities, or through quantum mechanical calculations.

The mass attenuation coefficients (μ/ρ)



M. Krause et al., "X-ray fluorescence cross sections for K and L X-rays of the elements", Oak Ridge National Laboratory, Report No.: ORNL-5399 (1978)

Several databases exist and some of them are accessible to the community: Berger[a] (available online (NIST-XCOM) or xraylib), Henke[b] (available online (CXRO)), Elam[c], Ebel[d], Cullen[e]. Unfortunately, large uncertainties are reported.

[a] M.J. Berger et al., XCOM: Photon Cross Sections Database. Available online: http://physics.nist.gov/PhysRefData/Xcom/Text/XCOM.html

[b] B.L. Henke et al., photoabsorption, scattering, transmission, and reflection at E=50-30000 eV, Z=1-92, Atomic Data and Nuclear Data Tables Vol. 54 (2), 181-342 (1993). Available online: http://henke.lbl.gov/optical_constants/

[c] W.T. Elam et al., A new atomic database for X-ray spectroscopic calculations, Radiation Physics and Chemistry, Vol. 63, pp. 121128, 2002

[d] H. Ebel et al., Numerical description of photoelectric absorption coefficients for fundamental parameters programs, X-Ray Spectrometry, vol. 32, no. 6, pp. 442451, 2003

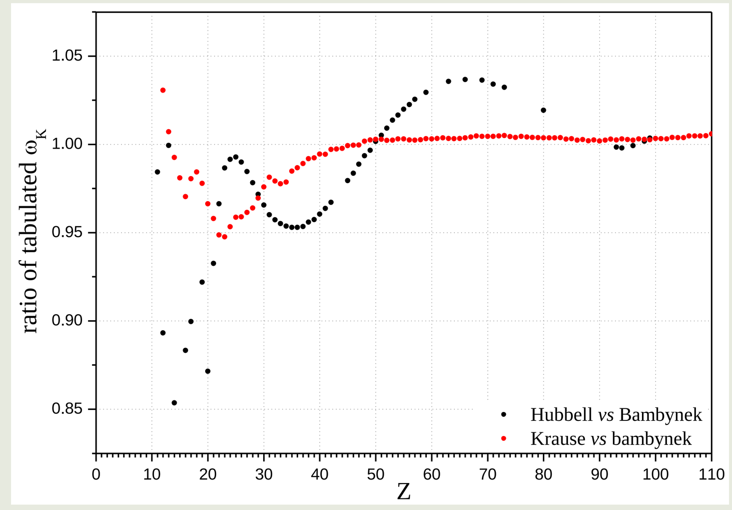
[e] Dermott E. Cullen, UCRL--50400, Vol. 6, Rev. 5; „EPDL97: the Evaluated Photon Data Library".

The fluorescence yields (ω)

The available databases contain only limited experimental results, together with theoretical calculations. Nonetheless, discrepancies exist between tables: see example between Bambynek[f], Krause[g] and Hubbell[h]

Estimated percentage uncertainties for fluorescence and Coster-Kronig yields

Z (range)	ω_K	ω_{L1}	ω_{L2}	ω_{L3}	f_{12}	f_{13}	f_{23}
5-10	40-10						
10-20	10-5	>30	>25	>25	10	5	
20-30	5-3	30	25	25	15	10	40
30-40	3	30	25	20	15	10	30-20
40-50	2	30-20	25-10	20-10	20	10	20
50-60	2-1	20-15	10	10-5	20	15	20
60-70	1	15	10-5	5	15	10	20-15
70-80	1	15	5	5-3	20	10-5	15
80-90	<1	15	5	3	10	5	15
90-100	<1	15-20	10	3-5	10-50	5-10	15
100-110	1	20	10	5	50-100	15	20



[f] W. Bambynek et al., Review of Modern Physics, Vol. 44 (1972)

[g] M.O. Krause, J. Phys. Chem. Ref. Data., Vol. 8 (1979)

[h] J.H. Hubbell et al., J. Phys. Chem. Ref. Data., Vol. 23 (1994)

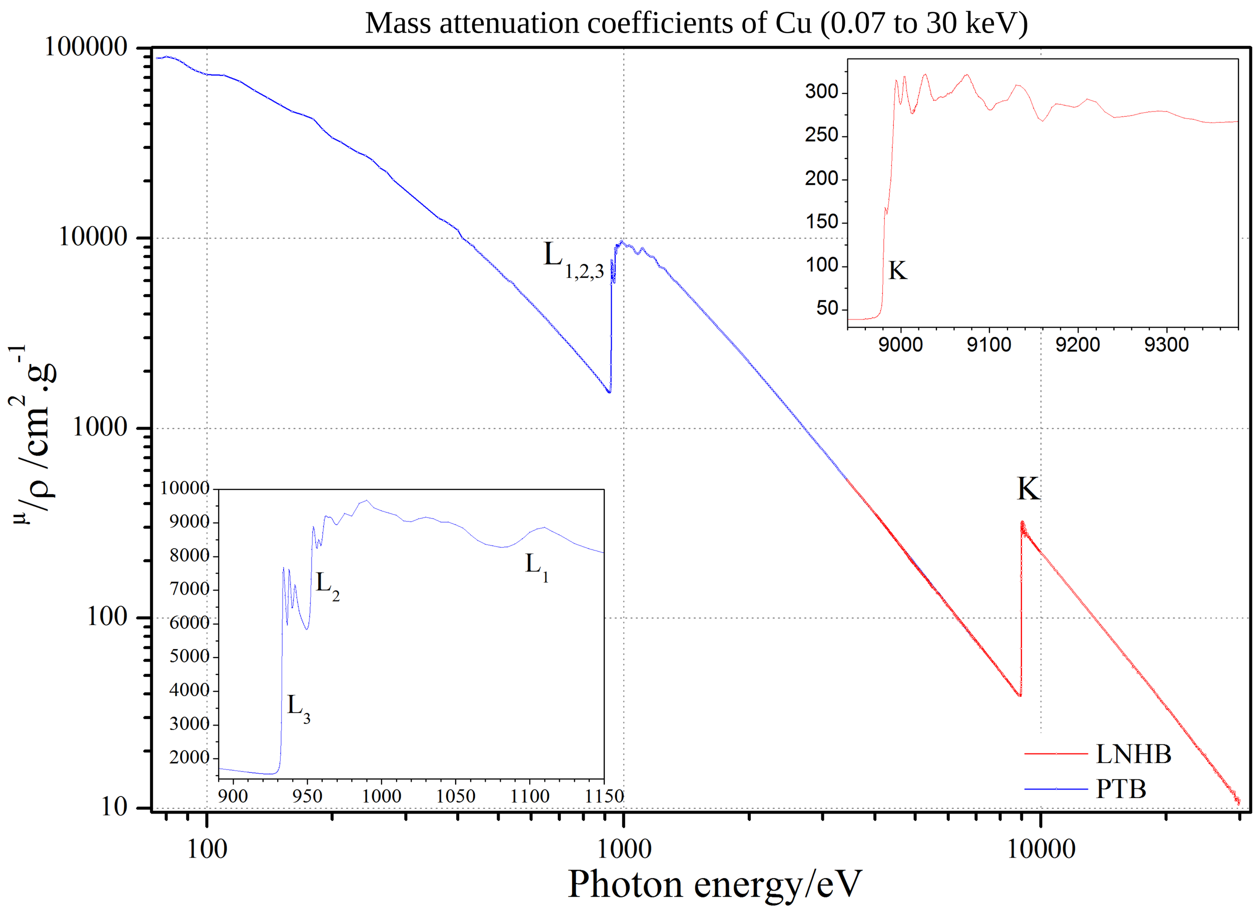
MEASUREMENT OF THE MASS ATTENUATION COEFFICIENTS OF Cu (LNHB & PTB)

Transmission measurement of thin samples: the Beer-Lambert law links the transmission to the total mass attenuation coefficient

$$\mu/\rho = -\frac{A}{M} \times \ln\left(\frac{I - I_{bruit}}{I_0 - I_{bruit}}\right) \times k_P$$

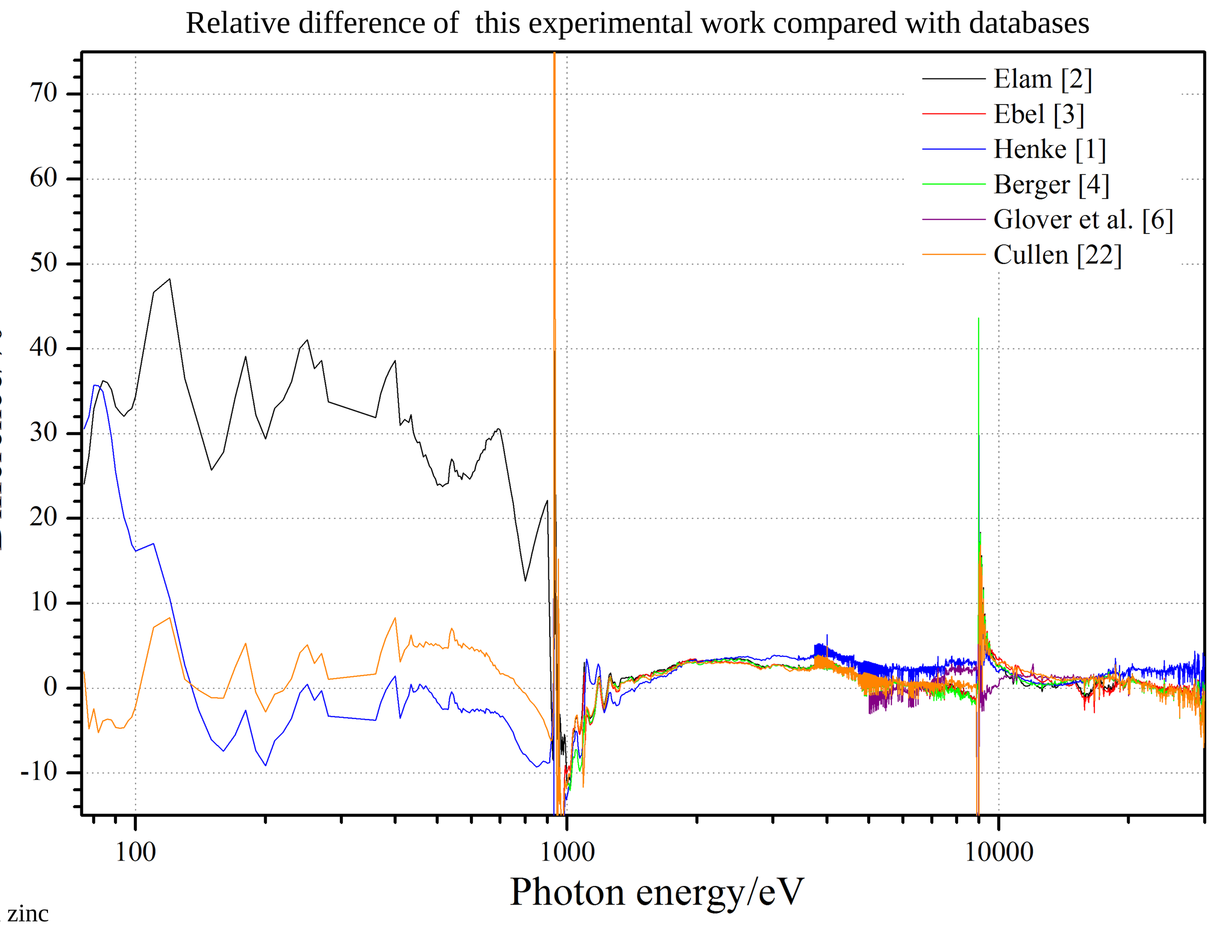
→ independent measurement of the sample mass (M) and area (A) is needed
→ evaluation of the bias introduced by possible elemental impurities (k_p)
→ special care was taken to characterize the photon beam (stability, monochromaticity, size)
→ careful evaluation of the combined standard uncertainty budget

Mass attenuation coefficients of Cu (0.07 to 30 keV)



Contribution to the total uncertainty budget	
Mass	$0.02\% < U_m < 0.3\%$
Area	$0.02\% < U_a < 0.05\%$
Area homogeneity	$U_H < 0.4\%$
Transmission measurement	$U_T \sim 0.2\%$
Purity	$U_P < 0.6\%$
Combined standard uncertainty	$0.5\% < U < 1.5\%$

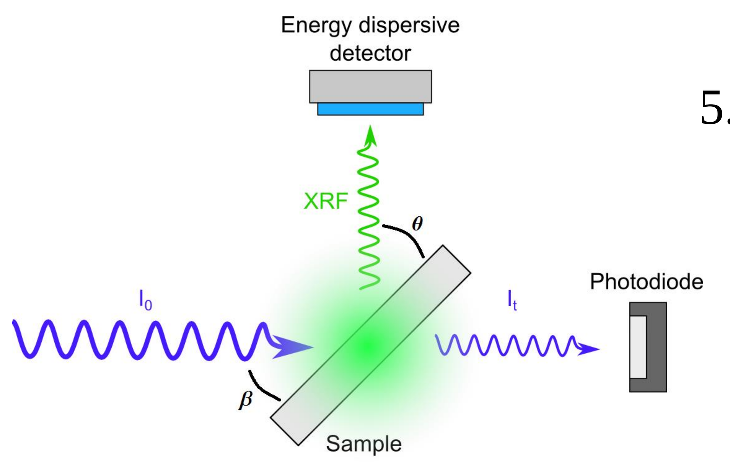
Relative difference of this experimental work compared with databases



More details in ► Y. Ménesguen et al., High accuracy experimental determination of copper and zinc mass attenuation coefficients in the 100 eV to 30 keV photon energy range, Metrologia **53** (2016) 7-17

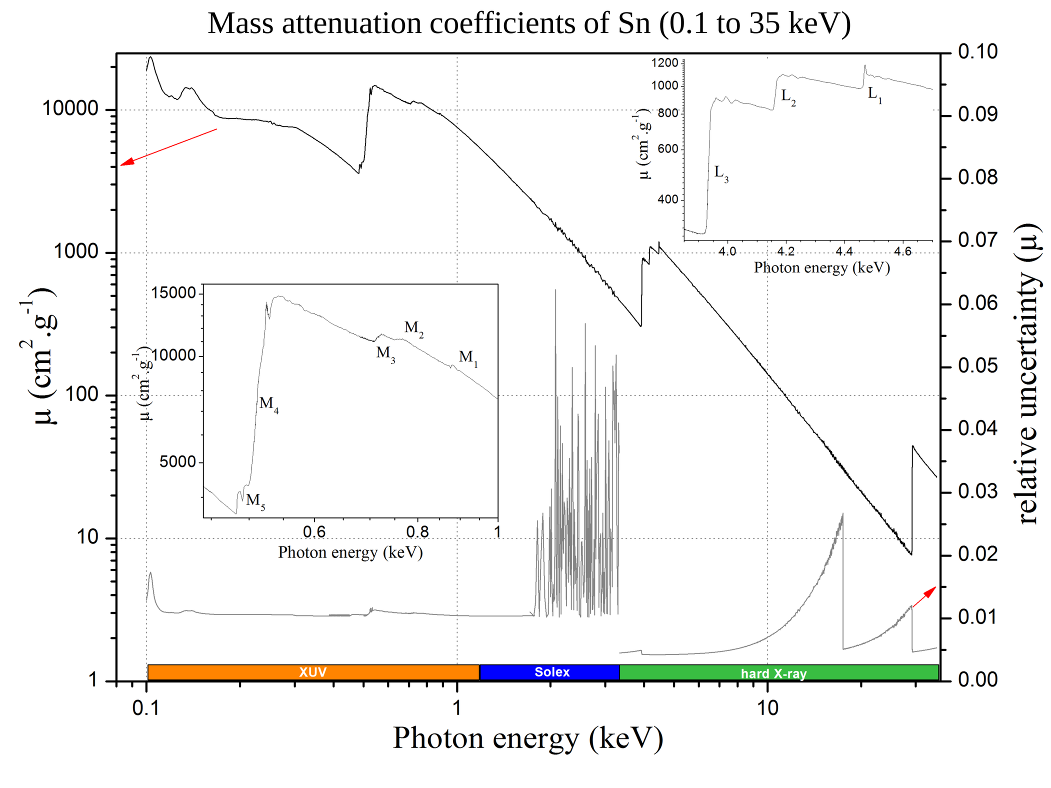
DETERMINATION OF μ, τ, ω, and f OF Sn

1. μ are measured by a transmission setup using samples of different thicknesses in the 0.1-35 keV energy range
2. Partial attenuation coefficients due to the L subshells are derived from μ
3. Fluorescence spectra are recorded as the excitation photon energy is progressively increased across each partial L transition edge

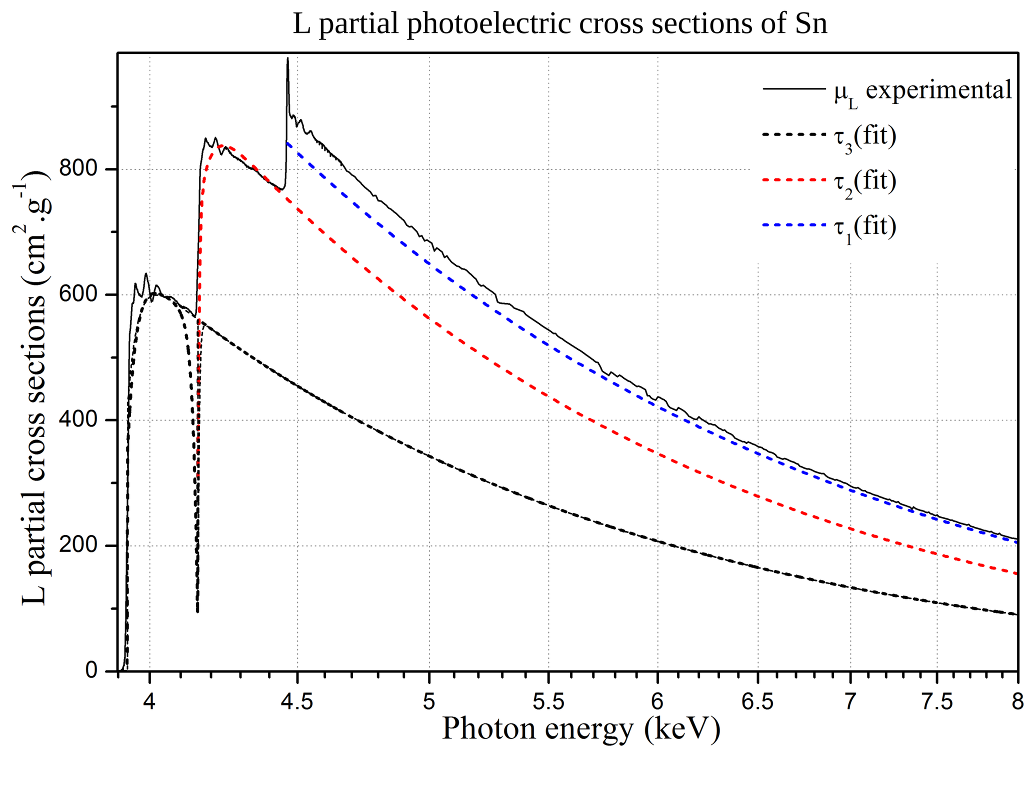


4. ω×τ are derived from fluorescence spectra using Sherman's equations
5. A fitting procedure is used to take into account the electron correlation effect on the photoabsorption coefficient (τ) near the transition energies, starting with the L_3 subshell to derive ω_3 and τ_3, which are then used to derive f_{23} with an excitation energy above L_2 …

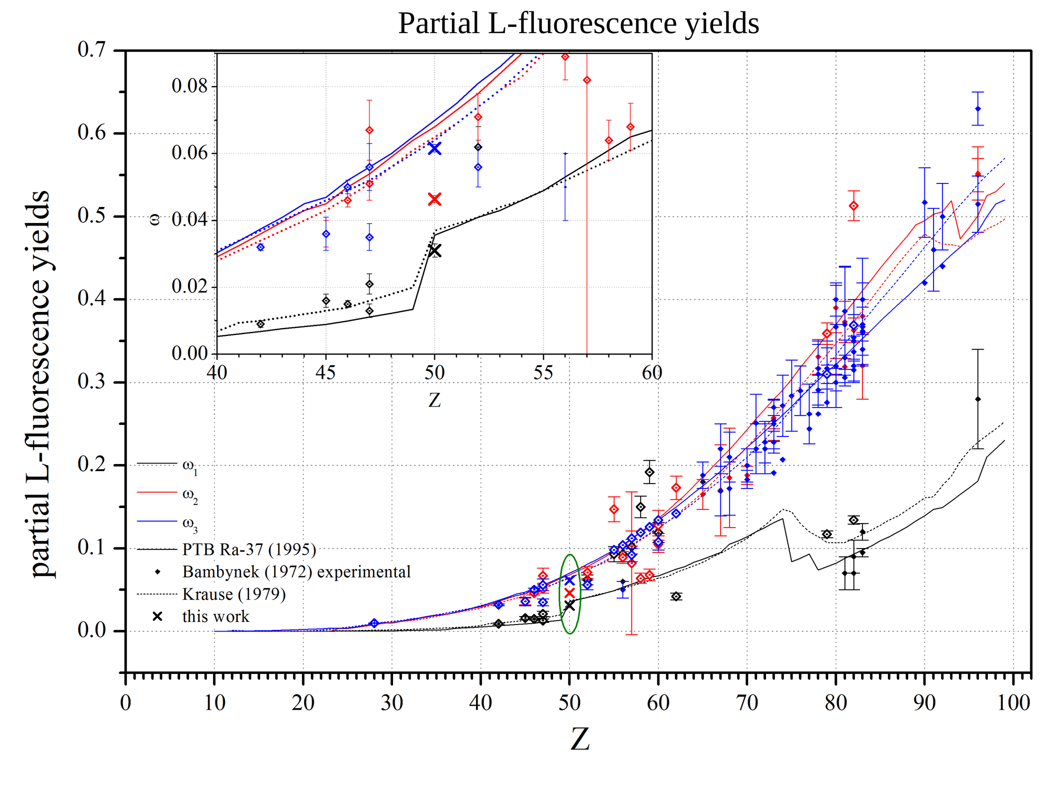
Mass attenuation coefficients of Sn (0.1 to 35 keV)



L partial photoelectric cross sections of Sn



Partial L-fluorescence yields



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