

## The Impact of Phase on Mass Absorption Coefficients Using Soft X-ray Emission Spectrometry

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Quantitative chemical analysis, an essential step in material development and characterization, remains a trying task due to the electron-matter interaction phenomena that affect acquired data. One such problem is X-ray absorption, where photons generated inside a material are absorbed by other atoms prior to exit [1]. The photon is absorbed and the energy is transferred to the orbital electron. This causes attenuations in the amount of X-rays exiting the surface and a discrepancy in the intensities detected. These discrepancies can be accounted for in simulations if the mass absorption coefficient (MAC) is known. MACs have been largely tabulated for the  $K\alpha$  lines of a wide range of elements [2]. However, with new capabilities for doing microanalysis and chemical quantification using soft X-rays at low accelerating voltages, MAC values for lower excitation energy lines must be known. At energies exciting the L, M, and N shells of materials, chemical bonding and effects within the band structure can come into play, increasing the complexity of determining the mass absorption contribution and constructing accurate simulation calculations [3]. Furthermore, this implies that such MAC values may also vary with phase composition and are not necessarily constant for each single element. Here, we investigate the contributions of these factors to the mass absorption calculation and provide a method for computing mass absorption coefficients of soft X-rays.

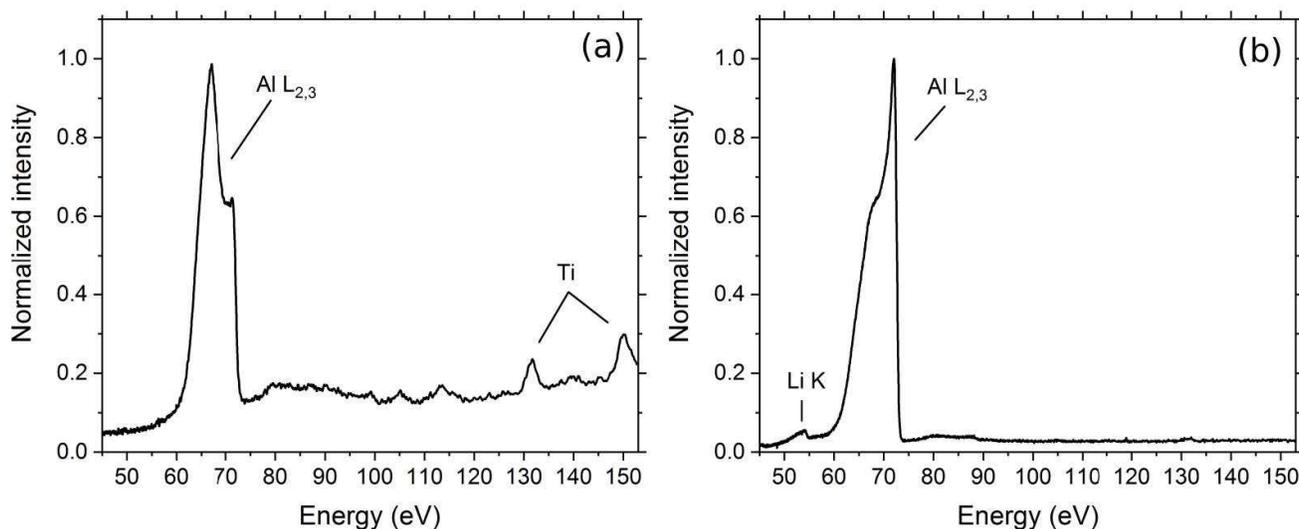
Experimental X-ray intensities of a number of aluminum alloys were obtained using a JEOL 8530 field emission microprobe equipped with a soft X-ray emission spectrometer (SXES). Acquisitions were performed at various accelerating voltages within the range of 1 to 15 kV. A least squares approach was used to fit the X-ray intensity function with absorption [3] to the integrated peaks. The integrated peak intensities were first normalized so as to eliminate the need for knowing the values of the instrument specific variables in the intensity equation. The intensity function does however require an integration of the depth distribution curve,  $\varphi(\rho z)$ . These curves are obtained by Monte Carlo modelling using the Monte Carlo software MC X-ray [4]. The cross-sections used in these simulations must take in to account the above mentioned low energy effects, and do so using additional parameters such as the Koster-Cronig factor [3].

The soft X-ray spectrum of TiAl at 3 kV is displayed in Figure 1 (a). The Al  $L_{2,3}$  and the 3<sup>rd</sup> order Ti  $L\alpha$  and  $L\alpha$  peaks are indicated, demonstrating the SXES detection capabilities within the soft X-ray range. The intensity spectrum of an Al-Li alloy UL40 (Al-0.04Li-0.018Zr) is depicted in Figure 1 (b), where the Li K peak, situated at approximately 55 eV is observed. The UL40 sample was prepared in an argon drybox and ion beam milled before analysis to remove oxygen and amorphous layers. The fitting method was first applied to compute the MAC of Li K in the Al-Li similar to previous work [5]. Figure 2 shows the experimentally obtained integrated intensities as a function of accelerating voltage as well as the fit of the X-ray intensity function obtained by the least squares calculation. The MAC value obtained was 11 527 g/cm<sup>2</sup>. This is in comparison to 8989 g/cm<sup>2</sup> obtained by the same method on a Li-Br com-

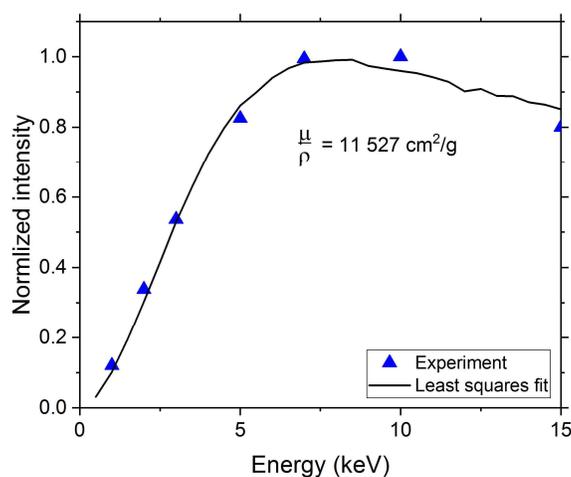
pound, indicating that crystal structure and phase composition may affect the mass absorption of elements, especially within the soft X-ray range.

#### References:

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**Figure 1.** SXES spectrum of (a) TiAl and (b) Al-Li alloy UL40 at 3 keV.



**Figure 2.** Least squares fit of X-ray intensity function to integrated Li peaks and computed MAC.