Quantitative XPS I: Analysis of X-ray Photoelectron Intensities from Elemental Data in a Digital Photoelectron Database

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An analysis of the correlation of theoretical predictions for photoelectron intensities is made with experimental data from an XPS digital database for 46 solid elements measured using a spectrometer with calibrated intensity and energy scales. This analysis covers spectral data for widescans at 1 eV intervals with kinetic energies from 200 eV to 1273 eV using Mg X-rays and to 1506 eV using Al X-rays, and also narrow scans around the photoelectron peaks at 0.1 eV intervals.

All spectra have the instrument intensity/energy response function removed so that the peak areas are proportional to the number of electrons emitted per steradian per incident $K\alpha$ photon. Correlations are made for the ionisation cross sections of Scofield and the inelastic mean free paths given by the TPP-2M formula. The correlations are excellent, apart from a factor which may be associated with the background removal arising from the use of the Tougaard Universal cross section. These correlations lead directly to pure element relative sensitivity factors suitable for quantitative analysis. General equations are also provided to extract values for a newly defined average matrix relative sensitivity factor (AMRSF). These AMRSFs lead to simpler equations involving matrix factors that are effectively unity instead of the traditional values in the range 0.3 to 3.0.

The equation for quantification is of the form:

$$X_A = \frac{F_A I_A / S_A}{\sum_i F_i (I_i / S_i)}$$

where, if S_A are the traditional pure element relative sensitivity factors (PERSFs), the distribution of matrix terms, F_i are shown in Fig 1 (b), whereas if the new AMRSFs are used, the distribution is shown in Fig 1 (a). The matrix terms in the latter case may be taken as unity and so the above equation reduces to the equation commonly used in commercial software systems. Use of the wrong traditional sensitivity factors leads directly to quantities that are in error by factors in the range 0.3 to 3.
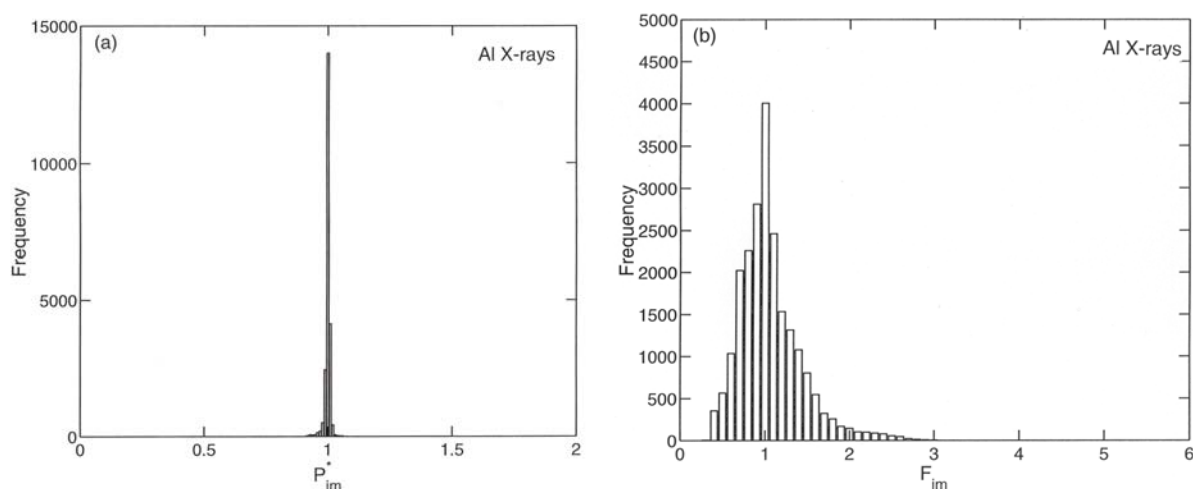
Fig 1 Populations of the matrix factors F_i for a species i in a matrix m given as: (a) P_{im}^* for AMRSFs and (b) F_{im} for PERSFs, for Al X-rays.