Supplementary Material

Pseudo Voigt fitting model.- Equation 1 explicitly shows all parameters involved; η stablishes the ratio between the Gaussian (left hand summand) and the Lorentzian (right hand summand) contributions to the profile $(0 < \eta < 1)$, λ_0 is the central wavelength of the line, and $\Delta\lambda_G$ and $\Delta\lambda_L$ are the full widths at half maximum (FWHM) of the Gaussian and the Lorentzian contributions, respectively. Since the pseudo-Voigt profile area is normalized to 1 [1], and the studied profiles did not fulfill this condition, a scale factor *K* accounting for the line intensity was added to the fitting model.

$$I(\lambda) = \left(\frac{2\sqrt{\ln 2}(1-\eta)}{\sqrt{\pi}\,\Delta\lambda_G} e^{-(\ln 2)\left(\frac{2(\lambda-\lambda_0)}{\Delta\lambda_G}\right)^2} + \frac{\eta\,\Delta\lambda_L}{2\pi\left[(\lambda-\lambda_0)^2 + \left(\frac{\Delta\lambda_L}{2}\right)^2\right]} \right) K$$

Equation 1

Bibliography

[1] M. Schmid, H. P. Steinrück, and J. M. Gottfried, "A new asymmetric Pseudo-Voigt function for more efficient fitting of XPS lines," *Surf. Interface Anal.*, vol. 46, no. 8, pp. 505–511, 2014.