

Theoretical derivation of the X-ray diffraction line profile based on its absorption

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Abstract: An X-ray diffraction line-profile is theoretically derived, based on the calculation of the superposition of absorbed X-ray wave reflecting by a perfect crystal. As the absorbed X-ray intensity is different by the distance it passing through, one obtain the total amplitude of the diffracting X-ray is $A_{Tot} = \sum_{n=0}^N A_n \exp(i\phi_n)$, where ϕ_n is the wave phase angle, and $A_n = \sqrt{I_0} \exp(-f(\mu s) n)$ is the decreased amplitude reflected by nth layer, s is the traverse distance between two crystallographic plane, μ is the absorption coefficient, and $f(\mu s)$ is the absorption function to be determinate. By simply assuming that the diffract intensity I is inversely proportional to μ , one can get an approximative expression for the profile, $I \approx \frac{I_0}{\mu s + \Delta\theta^2}$, which is just the Cauchy empirical fitting functions, where θ is the Bragg angle. Thus one obtains that the Cauchy function is just a special case of our theoretical result. Another verification is performed by experiment, Fig.1 shows both the experiment line profile and the theoretical one.

As the theoretical line profile is fairly close to that of the experiment result, one can conclude that the line profile is mainly shaped by the X-ray absorption, rather than by the instrumental broadening or by the specimen caused broadening.

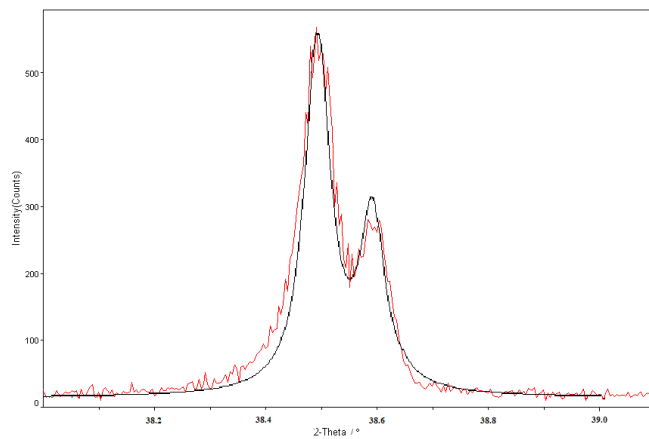


Fig.1. X-ray diffraction line-profiles of the experiment (red) and the theoretical (black) one for Aluminum powder (111) plane, with Copper (Cu) radiation $K_{\alpha 1}$ and $K_{\alpha 2}$.