EXPERIMENT VERIFICATION FOR THE DEPENDENCE OF THE X-RAY DIFFRACTION LINE PROFILE WITH THE ABSORPTION OF SAMPLE

Kejia Liu and Heifen Chen
School of Material Science and Engineering, Shanghai Institute of Technology,
Shanghai, China 200233

X-ray diffraction (XRD) provides a lot of information of the crystalline sample. One can obtain a lot of information about the micro-structure of the specimen by XRD line profile analysis. It was supposed that the line profile is broadened by the size of the crystalline, and also broadened by mal-designed instrument. We proposed recently, (Kejia Liu *et al*, Adv. X-ray analysis, V53, to be published) that there is still another effect which affect the line profile, that is, the absorption of the sample, and we obtained that the intensity of the XRD is,

$$I = I_0 \frac{1}{1+e^{-2\sqrt{\mu s}} - 2e^{-\sqrt{\mu s}} \cos(4\pi d \sin(\theta)/\lambda)}.$$

Where I_0 is the reflected intensity, θ is the Bragg's angle, λ is the wave length, d is the interplanar spacing, $s = 4d^2/\lambda$, and μ is the mass absorption coefficient of the sample. We showed in our paper mentioned above, that the observed aluminum powder XRD patterns are in excellent agreement with the calculated line profile functions derived from absorption as shown in above. In this work, we shall discuss the dependence of the line profile with the absorption coefficient in detail, and shall give some concrete experiment evidence to support the calculated results, a typical result is shown in Fig 1.

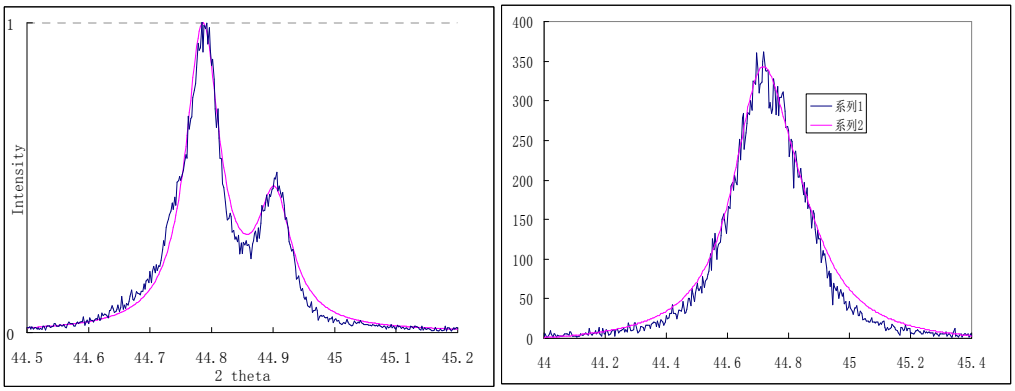

Fig 1. The power XRD line profiles for Aluminum (200) (left) and the Iron (110) plane (right), with copper doublet ($K_{\alpha 1}$ and $K_{\alpha 2}$) radiations. The Bragg's angles for two samples are near, and all of the other experimental conditions are the same. The difference between two calculated curve (red), which is caused by the absorption of the X-ray, and the experimental one (blue) are less than 10%. Therefore, the observed patterns for two different absorption samples are in good agreement with the calculated curves