Lorentz–polarization factor for correction of diffraction-line profiles. By WANG YINGHUA, Engineering Physics Department, Tsinghua University, Beijing, People’s Republic of China

Abstract
The Lorentz–polarization factor \((1 + \cos^2 2\theta)/\sin^2 \theta \cos \theta\) for the integrated intensity of a diffraction line is different from the Lorentz–polarization factor \((1 + \cos^2 2\theta)/\sin^2 \theta\) for a diffraction-line profile; nevertheless, in most of the literature it is being used to correct diffraction-line profiles. The errors introduced in the peak shape and position by use of the Lorentz–polarization factor \((1 + \cos^2 2\theta)/\sin^2 \theta \cos \theta\) are discussed.

Although Warren & Averbach (1950) have calculated expressions for diffraction-line profiles \(I(2\theta)\) for a cold-work distorted powder specimen, and Wilson (1963), Delhez, Mittemeijer, de Keijser & Rozendaal (1977), and Delhez, de Keijser & Mittemeijer (1980) referred to diffraction-line profiles and the Lorentz–polarization factor for correction of diffraction-line profiles, a detailed analysis of both factors and their effect on experimental results is not included in these articles. As a result, at present, the Lorentz–polarization factor for integrated intensity is still used in correcting for diffraction-line profiles in most books (e.g. Klug & Alexander, 1974; Fan Xiong, 1981), articles (e.g. Taira, Yoshioka & Sakata, 1965) and computer programs for stress measurements in present instruments. Although this method of correction does not produce any obvious errors in the range of small Bragg angles, the first factor quoted in the Abstract is no more convenient than the latter. Therefore, it does not simplify the calculations, and it seems to be through a confusion in the concepts that the Lorentz–polarization factor for correction of integrated intensity is applied to the correction of diffraction-line profiles.

An expression for the integrated intensity \(I_{\text{int}}\) is given for a powder specimen in textbooks (e.g. Guinier, 1963; Azaroff, 1968). For an unpolarized incident beam, the Lorentz–polarization factor is

\[
(1 + \cos^2 2\theta)/\sin^2 \theta \cos \theta;
\]

for convenience, this is hereafter denoted by \(L_p(1)\). On the other hand, generalization of the calculation for cold-worked distorted specimens by Warren & Averbach (1950) gives

\[
I_{\text{int}} = \int I(2\theta) \, d2\theta = K \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} \int \int \cos \theta L(s) \, ds_1 \, ds_2 \, d2\theta.
\]

Therefore, the formula for the Lorentz–polarization factor related to diffraction-line profiles is

\[
(1 + \cos^2 2\theta)/\sin^2 \theta.
\]

Thus

\[
I(2\theta) = K \frac{1 + \cos^2 2\theta}{\sin^2 \theta} \int \int L(s) \, ds_1 \, ds_2.
\]

This is denoted by \(L_p(2)\). The polarization factor is \((1 + \cos^2 2\theta)/2\) in both \(L_p(1)\) and \(L_p(2)\). We can show that it becomes \((1 + \cos^2 2\theta)/(1 + \cos^2 2\theta_0)\) (Wilson, 1970) when a monochromator is used in the incident beam, where \(\theta_0\) is the Bragg angle of the monochromator crystal. It is unity for synchrotron sources, because the directions of the acceleration of the electron and the X-ray beam are perpendicular.

Curves of \(L_p(1)\) and \(L_p(2)\) as functions of \(\theta\) are given in Fig. 1. It is obvious that they are very different, especially for high Bragg angles. Therefore they will yield different results when diffraction lines of high \(\theta\) are used in experiments, as in measurements of stress and lattice parameter. The effects of
both correction factors on peak positions are given in Table 1 for five diffraction lines, assuming Gaussian profiles and corresponding Bragg angles of an Al specimen (Cu Kα radiation); \( B_{1/2} \) is the full width at half maximum (FWHM) and \( \Delta 2 \theta \) is the difference in peak positions for the diffraction line corrected by both factors. The peak positions are defined by a three-point parabola fitting method.

The data show that peak-position errors can reach 0.05–0.14° when using \( L_p(1) \) to correct diffraction-line profiles for intermediate-width diffraction lines. Since the accuracy of the three-point parabola fit or experimental error is only 0.001° when using a normal diffractometer, the error introduced by the use of \( L_p(1) \) is far larger than the experimental one. Diffraction-line profiles corrected by \( L_p(1) \) and \( L_p(2) \) respectively are given in Fig. 2 for Bragg angles of 68.84° and 81.57°. It is clear that not only the peak position but also the diffraction-line shapes or symmetry are affected by both correction factors.

The effects of the correction factors on lattice parameters were investigated by the same method as employed for the peak positions. Corresponding line positions of the Al specimen (Cu Kα radiation) \( \Delta a \) are 0.0000, 0.0003 and 0.0009 Å when \( B_{1/2} \) is 0.2, 1.7 and 3.4° respectively, where \( \Delta a \) is the difference of lattice parameters for a specimen when the diffraction-line profiles are corrected by \( L_p(1) \) and \( L_p(2) \). Thus use of \( L_p(1) \) to correct diffraction-line profiles will give errors of about 0.0003 Å for the intermediate-width diffraction line of the Al specimen with Gaussian profiles.

Stress values were also measured for a copper alloy specimen (Cu Kα radiation, Hilger diffractometer); they are -22.95, -20.18 and -23.35 kg mm⁻² when the diffraction-line profiles are not corrected, or corrected by \( L_p(1) \) and \( L_p(2) \) respectively. The error in the stress value introduced by using \( L_p(1) \) is thus about 3 kg mm⁻².

The author thanks Professors M. Schlenker, H. D. Li, Pan Jinsheng and Liu Baixin for help and discussions.

References


