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The influence of different Student's *T* mosaic distributions on the extinction factor in mosaic crystals

Hua-Chen Hu

China Institute of Atomic Energy, PO Box 275 (18), Beijing 102413, People's Republic of China. Correspondence e-mail: hchu3310@gmail.com

During the preparation of versatile tables for the secondary extinction factor Y_μ of cylindrical and spherical mosaic crystals expressed as functions of the Bragg angle θ, absorption coefficient times radius $\mu\rho$ and reduced radius $\tau_0 = \sigma_0\rho$ [$\sigma_0 = (2\pi)^{1/2}Q/\eta$], or of θ, τ_0 and $\xi_0 = \mu/\sigma_0$, five kinds of Student's Tn probability functions $T1$, $T2$, $T3$, $T4$, $T\infty$ for describing the mosaic distribution of crystals have been tested. $T1$ is Lorentzian (L) and $T\infty$ is close to Gaussian (G). The influence of these different mosaic distributions upon the reflection power ratio, the integrated reflection power ratio (the area under the rocking curve) and the extinction factor Y_μ in cylindrical crystals has been thoroughly investigated. For a weakly absorbing cylindrical crystal with τ_0 = 30, the value of Y_μ for the $T2$ distribution turns out to be nearly two times the value for G, but the difference between these distributions becomes small when $\xi_0 > 1$. The L distribution has been found to be unsuitable for describing the mosaic distribution. The determination of different types of mosaic distribution from the rocking curves is discussed based on these results. Finally $T2$, $T4$ and the G distribution have been found to be acceptable for the calculation of secondary extinction factor tables for cylindrical and spherical crystals.

1. Introduction

The notations used here are the same as those in Hu (2003): η is the mosaic spread; μ is the linear absorption coefficient or absorption cross section per unit volume; ρ is the radius of a sphere or a cylinder; σ is the diffracting or coherent scattering cross section per unit volume, $\sigma = QW(\Delta\theta_0)$ where Q is the average scattering cross section per unit volume and $W(\Delta\theta_0)$ is the mosaic distribution as a function of the scattering angle; $\xi = \mu/\sigma$. The parameters σ and ξ at $\Delta\theta_0 = 0$ are defined as σ_0 and $\xi_0 = \mu/\sigma_0$; $\tau_0 = \sigma_0\rho$ is the reduced radius. G is the Gaussian distribution, L is the Lorentzian distribution.

The type of mosaic distribution in a real single crystal is an important parameter for both structure refinement and monochromator design. The mosaic distribution is not always isotropic (Coppens & Hamilton, 1970) and homogeneous (Mathieson & Stevenson, 1986).

Crystals with G and L mosaic distributions were assumed by Becker & Coppens (1974) in their extinction theory. Hu (2003) pointed out that the difference in secondary extinction factors for cylindrical crystals assuming rectangular, G and L mosaic distributions may be quite noticeable when ξ_0 (= μ/σ_0) < 2. Sabine (1988) mentioned for the first time that the extinction factor for a non-absorbing cylindrical crystal with L distribution is divergent for the Laue case and large τ_0.

In order to construct a set of tables comprising wide ranges of τ_0 and $\mu\rho$ ($0 < \tau_0 \leq 30$ and $0 < \mu\rho \leq 30$) the secondary extinction factors for cylindrical and spherical crystals with different mosaic distributions have been investigated, aiming at a proper description of real crystals.

The present work contains the introduction for the first time of the Student's T distribution as a versatile profile of the mosaic distribution, and its influence upon the reflection power ratio P_H/P_0 (RPR), the integrated reflection power ratio (IRPR, the area under the rocking curve) and the extinction factor.

2. Method

Several T mosaic distribution functions have been considered.

The general Student's T probability density function with degree of freedom n is

$$W = f(x|n) = \frac{\Gamma[(n+1)/2]}{\Gamma(n/2)} \frac{1}{(n\pi)^{1/2}} \frac{1}{(1+x^2/n)^{(n+1)/2}}. \qquad (1)$$

The mosaic distribution $W(\Delta\theta_0)$ for different degrees of freedom n (n is an integer) is obtained after transforming the parameter x into $\Delta\theta/\eta$:

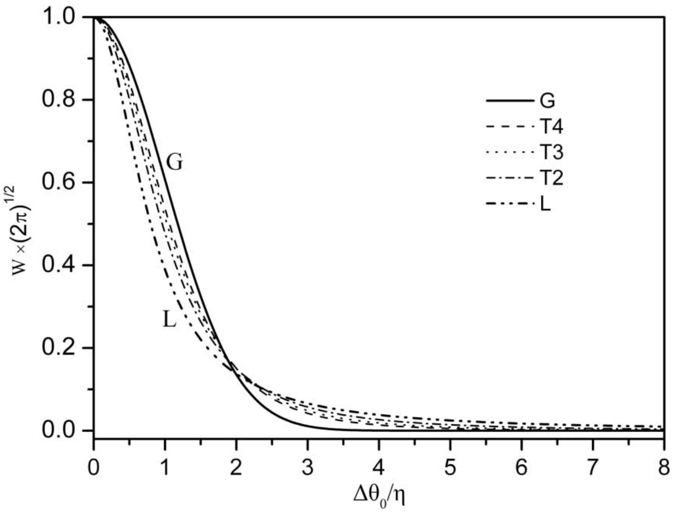

Figure 1
The Student's *Tn* probability density distributions $(2\pi)^{1/2}W$ as a function of $\Delta\theta_0/\eta$.

(1) Lorentzian distribution L (n = 1),

$$W(\Delta\theta_0) = [1/\eta(2\pi)^{1/2}][1 + \pi(\Delta\theta_0/\eta)^2/2]^{-1}; \qquad (2)$$

(2) $T2$ distribution (n = 2),

$$W(\Delta\theta_0) = [1/\eta(2\pi)^{1/2}][1 + (2/\pi)(\Delta\theta_0/\eta)^2/2]^{-3/2}; \qquad (3)$$

(3) $T3$ distribution (n = 3),

$$W(\Delta\theta_0) = [1/\eta(2\pi)^{1/2}][1 + (\pi/8)(\Delta\theta_0/\eta)^2]^{-2}; \qquad (4)$$

(4) $T4$ distribution (n = 4),

$$W(\Delta\theta_0) = [1/\eta(2\pi)^{1/2}][1 + (8/9\pi)(\Delta\theta_0/\eta)^2]^{-5/2}; \qquad (5)$$

(5) Gaussian distribution G ($n > 15$ or $\rightarrow \infty$),

$$W(\Delta\theta_0) = [1/\eta(2\pi)^{1/2}]\exp\{-[\Delta\theta_0]^2/2\eta^2\}. \qquad (6)$$

The FWHM values for L, $T2$, $T3$, $T4$ and G are 1.596, 1.921, 2.054, 2.125, 2.170 and 2.355 times η, respectively.

3. Results and explanations

Numerical results are presented for a cylinder of radius ρ. Fig. 1 shows the dependence of the *Tn* probability density function $(2\pi)^{1/2}W$ on $\Delta\theta_0/\eta$. Note the persisting tail of the Lorentzian distribution compared with $T2$, $T3$, $T4$ and G. Numerically, the fraction of the area of $(2\pi)^{1/2}W$ in the interval $-42 \leq \Delta\theta_0/\eta \leq 42$ is 0.9879, 0.9996, 0.9999 and 1.0 of the total area under the curve for L, $T2$, $T3$ and $T4$, respectively.

Fig. 2 shows the corresponding angular dependence of the RPR P_H/P_0 for cylindrical crystals with different mosaic distributions for ξ_0 = 0.016667, $\mu\rho$ = 0.5 and θ = 30°. The integrated reflection power ratio IRPR for the L distribution is even more persistent for large $\tau_0 = \sigma_0\rho$, as shown in Fig. 2. In fact, for large τ_0 the total area in the interval $-\infty \leq \Delta\theta_0/\eta \leq \infty$ diverges to infinity when ξ_0 is small enough.

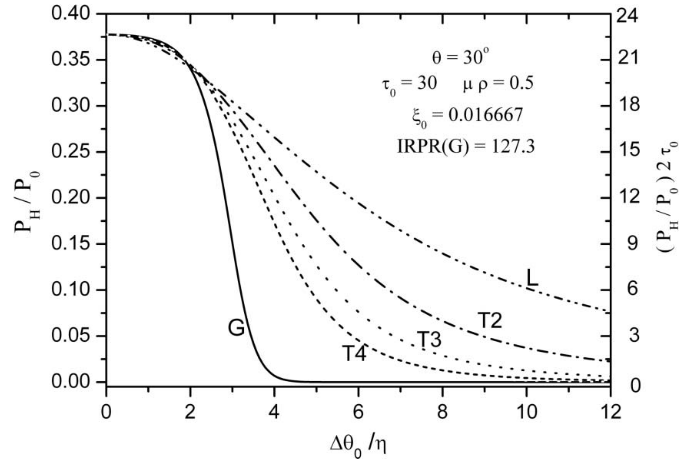

Figure 2
Rocking curves of RPR = P_H/P_0 and $2\tau_0 P_H/P_0$ for a cylindrical crystal with different mosaic distributions for ξ_0 = 0.016667, $\mu\rho$ = 0.5 and θ = 30°.

Figs. 3(*a*), 3(*b*) and 3(*c*) show the extinction factor Y_μ *versus* τ_0 for $\mu\rho$ = 0.5 and $\sin\theta$ = 0.15, 0.5 and 0.8, for four kinds of mosaic distribution L, $T2$, $T3$, $T4$. Y_μ has been evaluated with equations (3)–(18) of Hu (2003). For the L distribution $W'(\Delta\theta_0)$[1] is calculated with equation (2). It can be seen that a noticeable difference for different mosaic distributions begins to appear at τ_0 = 2.5 ($\xi_0 \leq 0.2$). The values of Y_μ in the integration interval $-42 \leq \Delta\theta_0/\eta \leq 42$ for L, $T2$, $T4$ and G are 0.1249, 0.0816, 0.0586 and 0.0402, respectively. Thus at τ_0 = 30 (ξ_0 = 0.016667) and $\sin\theta$ = 0.5, Y_μ for L, $T2$ and $T4$ is 3.11, 2.03 and 1.46 times larger than Y_μ for G, respectively. The corresponding RPR for $\sin\theta$ = 0.5 is shown in Fig. 2. The value of Y_μ for a weakly absorbing or non-absorbing cylindrical crystal with L distribution is divergent when the integration interval is $-\infty \leq \Delta\theta_0/\eta \leq \infty$. The value of Y_μ for the $T2$ distribution is 8.9% larger than the value for G even when τ_0 = 30, $\mu\rho$ = 30. For a sphere, the ratios of Y_μ for different distributions are quite similar to those for a cylinder.

Therefore, it seems that in real crystals the most reasonable mosaic distribution would be G, $T2$ or $T4$ but not L, and this will serve as a guideline for our calculation of extinction-factor tables.

It can be seen from Fig. 3(*d*) that a noticeable difference exists in the IRPR (*i.e.* the area under the rocking curve) for $\sin\theta$ = 0.15, 0.5 and 0.8 at τ_0 = 10. However, the related increase of Y_μ with $\sin\theta$ is less pronounced as shown in the curves highlighted by small circles in Figs. 3(*a*), 3(*b*) and 3(*c*). The reason for this is that, from the definition of Y_μ in Hu (2003), the absorption-correction factor A in the denominator of Y_μ also increases with increasing $\sin\theta$.

[1] $W'(\Delta\theta_0) = 1.012\, W(\Delta\theta_0)$ if $|\Delta\theta_0| \leq 42\eta$; and 0 otherwise. The total area under the curve for L of Fig. 1 within the interval $-\infty \leq \Delta\theta_0/\eta$ is equal to 1.

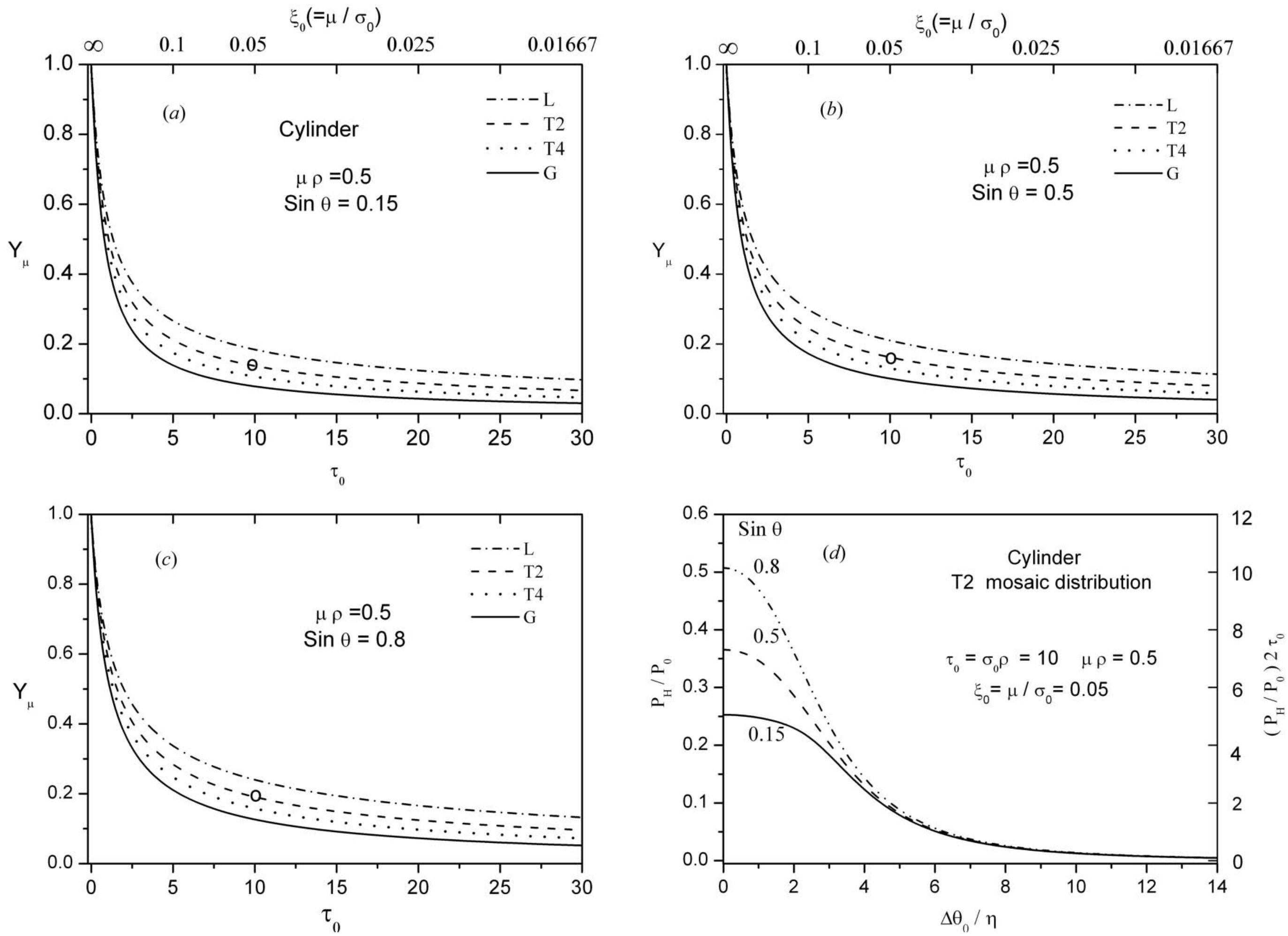

Figure 3
(*a*)–(*c*) Comparison of the extinction factor Y_μ for cylindrical crystals with four kinds of mosaic distribution as a function of τ_0 with $\mu\rho = 5$. (*a*) $\sin\theta = 0.15$; (*b*) $\sin\theta = 0.5$; (*c*) $\sin\theta = 0.8$. (*d*) Rocking curves of P_H/P_0 and $2\tau_0 P_H/P_0$ for a cylindrical crystal with $T2$ mosaic distribution at different values of $\sin\theta$, $\tau_0 = 10$.

4. Discussion

The relationships between RPR, Y_μ and θ, ξ_0, τ_0 for plane and cylindrical crystals have been investigated in detail by Hu (1997*a*,*b*, 2003).

According to the definition of the secondary extinction factor Y_μ expressed by equation (18) in Hu (2003), the physical meaning of Y_μ is the ratio between the IRPR resulting from multiple reflections and absorption within the crystal, and the IRPR due to a single reflection described by the kinematical approximation ($\mathrm{IRPR_k}$). This means that the measured rocking curve will resemble the intrinsic mosaic distribution only for $Y_\mu > 0.95$, implying that the IRPR is very close to the $\mathrm{IRPR_k}$. Such a condition may be satisfied only for the following cases:

(i) A thin non-absorbing or weakly absorbing crystal and $\tau_0 < 0.05$. Physically this means that the size of the crystal is far smaller than the diffraction mean free path (m.f.p.) of this crystal, so the RPR is smaller than 0.05 and the IRPR is close to $Qt\,\mathrm{cosec}\,\theta_0$ (θ_0 is the angle of incidence) for a plane crystal of thickness *t*, and close to QV for cylindrical and spherical crystals with volume *V*.

(ii) A thick crystal with $\xi_0 > 20$. The absorption m.f.p. for the crystal is much smaller than the diffraction m.f.p., so the RPR is smaller than 0.025. This condition is generally met in X-ray diffraction.

For a plane mosaic crystal of infinite thickness under Bragg geometry, the relationship between IRPR or Y_μ and ξ_0 has been thoroughly investigated by Hu (1997*a*,*b*). The author has pointed out that, for large ξ_0, the IRPR is close to

$$\mathrm{IRPR} = Q/(1-b)\mu$$

where *b* is the asymmetry parameter. In this case Y_μ is close to 1.

The properties of rocking curves from plane and cylindrical crystals have been investigated in Hu (1997*a*, 2003). It has been found that the FWHM of the rocking curve diminishes as ξ_0 increases at constant $\sigma_0 t\,\mathrm{cosec}\,\theta_0$ or τ_0.

After application of instrument corrections, the experimentally measured rocking curve represents the intrinsic mosaic distribution only if either condition (i) or (ii) is met. In cases different from (i) and (ii), for crystals with even, homogeneous mosaic distributions, a fit using an RPR obtained by solving Darwin's equations for each rocking angle would be necessary for obtaining the intrinsic mosaic distribution from the measured rocking curve.

Alianelli *et al.* (2004) have measured several rocking curves for different reflections from a flat copper crystal using 120 keV X-rays, and have obtained a rather satisfactory fit using a mixed mosaic distribution with 60% L and 40% G (see Fig. 9 of their paper). This further proves the necessity for describing the mosaic of a single crystal with a distribution intermediate between G and L.[2]

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[2] However their nomenclature 'QW-secondary extinction coefficient' and 'secondary extinction depth' is misleading.