

## Compton Downscattering Corrections to the Crystal Monochromator Efficiency\*

BY NIGEL J. SHEVCHIK†

*Division of Engineering and Applied Physics, Harvard University, Cambridge, Mass. 02138, U.S.A.*

(Received 26 January 1973; accepted 10 May 1973)

It is shown that when both a characteristic line of the X-ray spectrum and its nearby continuum are incident on the sample, the crystal monochromator efficiency derived by Ruland is decreased.

In a radial distribution analysis, small corrections in the experimental scattered X-ray intensity become important when the data are extended to high  $k$  values, where not only does the intensity fall, but so does the relative magnitude of the information-carrying oscillations. These corrections become particularly crucial when the high-angle-normalization method is used, since important quantities of the radial distribution function, such as the density and coordination number, depend directly on the accuracy of the normalization.

Use of a crystal monochromator in the diffracted beam does not guarantee that Compton processes at high angle can be neglected. Although the monochromator is effective in removing the Compton scattering produced by the energy band to which it is tuned, it is less effective in removing Compton-scattered radiation produced from the high-energy shoulder of the incident beam.

An estimate of the 'Compton downscattering' contribution to the observed intensity necessitates knowledge of  $E(\lambda)$ , the intensity of the incident beam as a function of the wavelength. The incident beam wavelength profile can, in general, be approximated, as is shown in Fig. 1, by a sharp peak of height  $E_0$  and of width  $\Delta\lambda_0$ , and a flat shoulder lying at wavelengths shorter than  $\lambda_0$  with a height  $E_s$ . We ignore the part of the continuum that lies at longer wavelengths, since we do not expect the Compton scattering produced in this range to pass through the monochromator. In normal diffraction experiments,  $\lambda_0$  is the wavelength, usually a characteristic line in the X-ray spectrum, to which the monochromator is tuned. The shoulder has a cut off at  $\lambda_1$  which arises either from a cut off in the excitation energies of the electrons incident on the anode of the X-ray tube, or from the use of a metal filter in the incident beam.

Following Ruland (1964) the Compton profile, *i.e.* the distribution of wavelengths of the modified scattered radiation, produced by a delta-function in-

cident beam of wavelength  $\lambda'$  can be represented by a profile function of form:

$$\frac{1}{\Delta\lambda} h \left( \frac{\lambda - \lambda' - \Delta\lambda_C}{\Delta\lambda} \right) \quad \text{for } \lambda > \lambda' \\ 0 \quad \text{for } \lambda < \lambda', \quad (1)$$

where  $\Delta\lambda_C$  is average change in the photon wavelength and  $\Delta\lambda$  is the width of the Compton profile (Ruland, 1964). Note that this distribution is zero for wavelengths less than that of the incident beam. This is because it is unlikely from conservation of energy for a scattered photon to have more energy than the incident photon. We take the profile distribution to be normalized so that

$$\frac{1}{\Delta\lambda} \int_{-\Delta\lambda_C}^{\infty} h \left( \frac{u}{\Delta\lambda} \right) du = f_{\text{inc}}(k) \quad (2)$$

where  $f_{\text{inc}}(k)$  is the Compton scattering factor for the material under investigation and  $k$  is the total momentum transfer between the incident and scattered photons.

The total Compton intensity per unit wavelength downscattered from the white-radiation shoulder to wavelength  $\lambda_0$  is given by:

$$E_{CD}(\lambda_0) = E_s \int_{\lambda_1}^{\lambda_0} \frac{1}{\Delta\lambda} h \left( \frac{\lambda_0 - \lambda' - \Delta\lambda_C}{\Delta\lambda} \right) d\lambda' \\ = E_s \int_{-\Delta\lambda_C}^{\lambda_0 - \Delta\lambda_C - \lambda_1} \frac{1}{\Delta\lambda} h \left( \frac{u}{\Delta\lambda} \right) du. \quad (3)$$

For any profile function which decays with wavelengths away from the center of the profile, and for which the integral has converged at the upper limit, the profile width and position are lost in the integration and we have the simple result that the total downscattered Compton radiation is:

$$E_{CD}(\lambda_0) = E_s f_{\text{inc}}(k). \quad (4)$$

However, if the integral has not converged, such as in the case where  $\lambda_0 - \lambda_1 - \Delta\lambda_C \sim \Delta\lambda$ , we can approximate the long wavelength side of the distribution with a

\* Work supported by ONR, ARPA and DEAP.

† Present address: Max-Planck-Institut für Festkörperforschung, 7000 Stuttgart, Germany (BRD).

Lorentzian. The total downscattered Compton intensity per unit wavelength becomes for  $\lambda_0 - \Delta\lambda_c - \lambda_1 > \Delta\lambda_c$ :

$$E_{CD}(\lambda_0) = E_S f_{inc}(k) \left\{ \frac{1}{2} + \frac{1}{\pi} \tan^{-1} \left( \frac{\lambda_0 - \Delta\lambda_c - \lambda_1}{\Delta\lambda} \right) \right\}. \quad (5)$$

The total observed downscattered intensity,  $I_{CD}(k)$ , is approximately the downscattered Compton intensity per unit wavelength evaluated at  $\lambda_0$  times the monochromator bandpass width,  $b$ , or:

$$I_{CD}(k) = b E_{CD}(\lambda_0). \quad (6)$$

To obtain the total observed incoherent intensity, we must also consider the incoherent intensity arising from the characteristic line. The total Compton scattered intensity produced by the peak at  $\lambda_0$  is  $f_{inc}(k) E_0 \Delta\lambda_0$ , but the observed intensity is decreased by a factor  $O(k)$ , the monochromator efficiency (Ruland, 1964). Hence, the total observed incoherent Compton scattered intensity is the sum of these two components, or:

$$I_C(k) = Q(k) E_0 \Delta\lambda_0 f_{inc}(k) + b E_S f_{inc}(k) \times \left\{ \frac{1}{2} + \frac{1}{\pi} \tan^{-1} \left( \frac{\lambda_0 - \Delta\lambda_c - \lambda_1}{\Delta\lambda} \right) \right\}, \quad (7)$$

which can be written in the more convenient form:

$$I_C(k) = E_0 \Delta\lambda_0 f_{inc}(k) (Q(k) + CD) \quad (8)$$

where

$$CD = \frac{E_S b}{E_0 \Delta\lambda_0} \left\{ \frac{1}{2} + \frac{1}{\pi} \tan^{-1} \left( \frac{\lambda_0 - \Delta\lambda_c - \lambda_1}{\Delta\lambda} \right) \right\}. \quad (9)$$

Under usual operating conditions, the argument of the arctangent term is large, and

$$CD \simeq \frac{E_S b}{E_0 \Delta\lambda_0}. \quad (10)$$

In this case, the term  $CD$  is simply the ratio of the total power from the continuum contained in segment of length  $b$  to the total power in the characteristic line.

The net effect of this downscattering contribution is to make the monochromator less efficient by adding to  $Q(k)$  an almost constant term,  $CD$ . As long as the band pass,  $b$ , is wider than  $\Delta\lambda_0$ , this contribution becomes smaller with decreasing  $b$ . If the incident beam is monochromatic, the downscattering does not enter; however, the loss in intensity required to make the incident beam monochromatic may not be worthwhile. In some cases, it may be better to maintain the full intensity of a polychromatic incident beam and make this correction to the data.

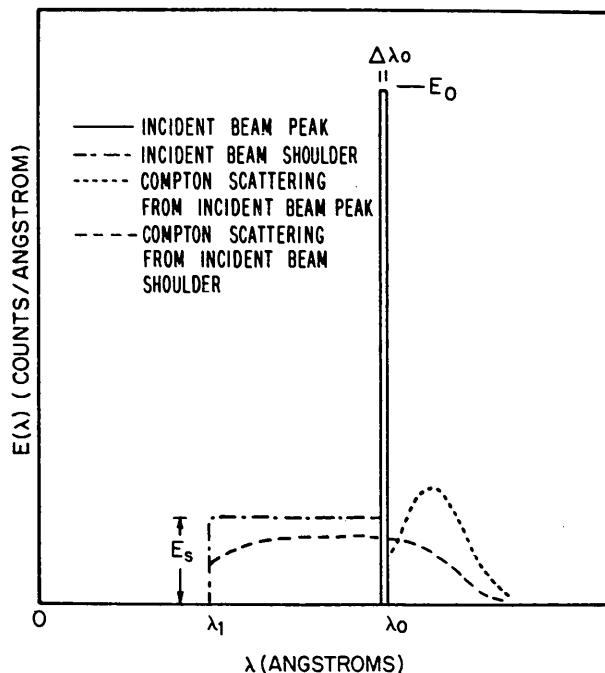


Fig. 1. The incident beam and Compton-scattered wavelength profiles.

The magnitude of the constant  $CD$  can be estimated by examining an experimentally determined wavelength distribution emitted from an X-ray tube under normal operating conditions. Such spectra are shown in *International Tables for X-ray Crystallography* (1962). We find that the power from the continuum contained in a segment of a length typical for a monochromator bandpass ( $b = 0.02 \text{ \AA}$ ) is  $\sim 10\%$  of the energy in  $K\alpha_{1/2}$  doublet, thus  $CD \sim 0.1$ . For large scattering vectors ( $k \sim 15 \text{ \AA}^{-1}$ ), this compares with the value of  $Q(k) = 0.2$  in this range deduced from Ruland's curves. Thus, the Compton downscattering effect is about 50% of the value of  $Q(k)$  and cannot be neglected. When using X-ray tubes that are contaminated by the tungsten filament, the ratio of the continuum to the  $K\alpha$  component is increased, making downscattering corrections even more important.

#### References

- International Tables for X-ray Crystallography* (1962). Vol. I. Birmingham: Kynoch Press.  
RULAND, W. (1964). *Brit. J. Appl. Phys.* **15**, 1301.