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A method of distinguishing between Gauss and Cauchy diffraction profiles. By G. B. Mitra,
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The Warren–Averbach (1950) method of Fourier coefficients for determination of particle size and strain in aggregates of distorted crystallites requires a knowledge of the strain profile. There is, however, considerable controversy regarding the nature of this profile, one school of thought favouring the Gauss type (*e.g.* Warren, 1959) the other favouring the Cauchy type (*e.g.* Williamson & Smallman, 1954; Wilson, 1958). This problem can be studied experimentally only by investigating the observed diffraction profiles. The observed line profile (obtained after eliminating the effects of geometrical profile) is a convolution of the particle-size profile and the strain profile. Hence, if both the particle-size and strain profiles are of the Gauss type, the observed line profile will be of the Gauss type. Similarly if both are of the Cauchy type, the observed profile will also be of the Cauchy type. If either or both belong to some other form or if one belongs to the Gauss type and the other is of the Cauchy type, the observed line profile becomes more complicated. Experimental work (*e.g.* Schoening, Van Niekerk & Haul, 1952) seems to indicate that the last conjecture is not impossible. Whatever may be the exact nature, the observed profile must belong to some near-Gaussian type. In course of the present investigation, a method has been developed to ascertain whether the observed profile belongs to either Gauss or Cauchy type. Consideration of other types will be given at a later date.

One way of ascertaining the nature of the line profile is by direct curve fitting. But the difference between the Gauss type, the Cauchy type and other similar near-Gaussian distributions is rather difficult to determine by any direct numerical or graphical method. Hence it is necessary to develop some other technique which will make the difference between the functions more distinct. In this connection, it is worthwhile to note that even if the differences between the direct distributions are not appreciable, the differences between the corresponding cumulative distributions are much more prominent. This distinctive characteristic of cumulative distributions has been found useful in distinguishing between centrosymmetric and non-centrosymmetric space groups. The present work has utilised this distinguishing property of the cumulative distribution to decide whether a given line profile belongs to the Cauchy or the Gauss type.

Suppose that the intensity distribution of the line under study about the Bragg angle θ_0 is given by $I(\theta)$. The angles at which the intensity merges in the background are θ_1 and θ_2 respectively. Since both the Cauchy and Gauss distributions are symmetrical, $\theta_0-\theta_1=\theta_2-\theta_0=N$ (say). Let σ be the standard deviation of the distribution and let $x=(\theta-\theta_0)/\sigma$ be the new variable for the angular spread. Let us introduce a scale factor C, so that

$$CI(\theta)=F(\theta) \text{ and } \int_{-N/\sigma}^{+N/\sigma} F(x)dx=1 \; .$$

In terms of the new variable x the distribution has been denoted as $F(x)$. The cumulative distribution is defined by

$$R(x)=\int_0^x F(x)dx \; .$$

Then, for the Gaussian distribution $R(x)=\frac{1}{2}\operatorname{erf} x/\sqrt{2}$, and for the Cauchy distribution, $R(x)=(1/\pi)\tan^{-1}x$. Since we are investigating the nature of the curve between the cut-off values at $\pm N/\sigma$, all discussions regarding the very long tails of the Cauchy distribution bringing in singularities are precluded from our standpoint.

Fig. 1 shows plot of $R(x)$ versus x for Gauss and Cauchy profiles along with the experimentally evaluated $R(x)$ values for several lines of cold-worked and annealed filings of spectroscopically pure copper obtained with monochromatized Cu $K\alpha$-rays and manually operated diffractometer technique. It is observed that none of the line profiles can be said to belong entirely to either Gauss or Cauchy type.

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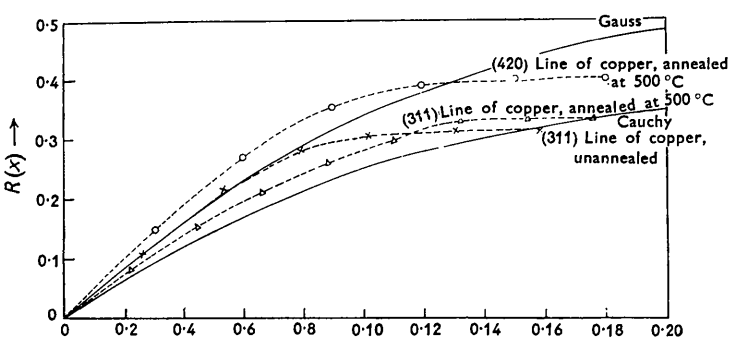

Fig. 1.