Correction of Measurements of Low-Angle X-Ray Scattering

It has been recognized that for accurate measurements of small-angle scattering it is necessary to use a monochromator. The monochromatized beam may have a very small width, but has a finite height which cannot be reduced without making the intensity of the beam too weak. If the intensity scattered at angle ϵ is $i(\epsilon)$, experiment does not give directly $i(\epsilon)$,

but $I(\epsilon) = 2 \int_0^A i \left(\sqrt{\epsilon^2 + \frac{t^2}{D^2}} \right) dt$; where A is the half-

height of the beam, D the distance between sample and film, and t the distance between one point of the beam and the plane of symmetry. For any value of A , the difference between $i(\epsilon)$ and $I(\epsilon)$ becomes important below a given value of ϵ . If $I(\epsilon)$ is practically zero for $\epsilon > \epsilon_0$ and if $A > D\epsilon_0$, $I(\epsilon)$ may be written more simply:

$$I(\epsilon) = 2 \int_0^\infty i \left(\sqrt{\epsilon^2 + \frac{t^2}{D^2}} \right) dt. \quad (1)$$

The approximate formula for i^1 is

$$i(\epsilon) = \text{const.} \exp \left(-\frac{4\pi^2 R^2 \epsilon^2}{3\lambda^2} \right), \quad (2)$$

where R is the radius of gyration of the diffracting particles and λ the wave-length of the incident radiation. If this particular function is put in formula (1), it is found² that:

$$I(\epsilon) = \frac{\sqrt{3}}{4\sqrt{\pi}} \cdot \frac{\lambda D}{R} i(\epsilon). \quad (3)$$

But formula (2) is only valid for small values of ϵ , and the integral (1) involves the whole exponential function. Thus, the result (3) is not correct.

Fig. 1

We have calculated the rigorous function $i(\epsilon)$ for spherical and ellipsoidal (axial ratio = v) particles of the same radius of gyration R . Then we calculated the corresponding functions $I(\epsilon)$. The result is that the approximate exponential form for $I(\epsilon)$ is not the same as for $i(\epsilon)$; the curve (Fig. 1) gives the calculated radius of gyration from $I(\epsilon)$ according to (3), and shows that the error is 3.5 per cent for spherical particles but grows very large for plate-shaped and particularly needle-shaped particles. It

can be shown, also, that the error is important in the case of mixtures of almost spherical particles of various diameters.

To obtain the corrected function $i(\epsilon)$, Shull and Roess³ decomposed the experimental function I into a sum of exponentials:

$$I = \sum_m C_m \exp(-m^2 \epsilon^2).$$

Then, according to (1),

$$i = \sum \frac{m C_m}{\sqrt{\pi} D} \exp(-m^2 \epsilon^2).$$

But this decomposition is not possible in every case, for example, for patterns with rings of very small diameter⁴.

There exists a general method of solving equation (1) (the calculation is due to MM. Bouzitat and Germain, of the Office National de Recherches Aéronautiques). The result is as follows:

$$i(\epsilon) = -\frac{1}{\pi D^2} \int_0^\infty \frac{I' \left(\sqrt{\epsilon^2 + \frac{u^2}{D^2}} \right)}{\sqrt{\epsilon^2 + \frac{u^2}{D^2}}} du; \quad (4)$$

(u is the integration parameter).

Fig. 2. —, curve a; ---, curve b; ·····, curve c

To use (4), it is necessary to determine the derivative $I'(\epsilon)$ from the experimental data. In order to check the accuracy of the method in a practical case, we considered the case of a schematic ring (Fig. 2 a), and we calculated the curve which would be observed with a beam of infinite height (Fig. 2 b). Then we determined graphically $i(\epsilon)$ from curve 2 b by means of the equation (4). The curve obtained (Fig. 2 c) is in satisfactory agreement with the theoretical curve.

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¹ Guinier, A., *Ann. Phys.*, **12**, 192 (1939).

² Hoseman, Z. *Elektrochem.*, **46**, 535 (1940).

³ Shull, C. G., and Roess, L. C., *J. Appl. Phys.*, **18**, 304 (1947).

⁴ Riley, D. P., "The Ultra-Fine Structure of Coals and Cokes", Brit. Coal Util. Res. Assoc., 232 (London, 1944). Guinier, A., *J. Chim. Phys.*, **40**, 133 (1943).