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Relation between particle sizes and strains determined by line-shape analysis on Gauss and Cauchy strain distribution hypotheses. By G. B. MITRA, *Department of Physics, Indian Institute of Technology, Kharagpur, India*

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Several authors (*e.g.* Michell & Haig, 1957; Michell & Lovegrove, 1960) have determined particle size and strain in deformed metals by the method of line-shape analysis on the basis of both Gauss and Cauchy strain distribution hypotheses. Their findings, generally, are:

(*a*) That the strain determined on the basis of Cauchy strain distribution hypothesis is 1·5 to 2 times as large as the strain determined assuming a Gaussian strain distribution.

(*b*) That the particle size determined on the basis of Cauchy hypothesis is several times as large as that determined assuming Gaussian distribution of strain.

These results call for a theoretical examination of the two relations.

Let A_n be the nth Fourier coefficient of the line profile of an *hkl* reflexion which has been converted into a $00l$ reflexion by suitable change of axes. Let s_g and s_c be the root-mean-square strains obtained on the basis of Gaussian and Cauchy strain distributions respectively and A^P_{ng} and A^P_{nc} be the nth order Fourier coefficients of the particle size profile obtained on the basis of the two distributions respectively. Then we may write

$$A_n = A^P_{ng}\exp\left(-2\pi^2l^2n^2s_g^2\right) \quad (1)$$

$$= A^P_{nc}\exp\left(-\pi^2(ln/\sigma)s_c^2\right) \quad (2)$$

where σ is the cut off value of the strain in the Cauchy strain profile. Differentiating equations (1) and (2), we have

$$\frac{dA_n}{dn} = \frac{dA^P_{ng}}{dn}\exp\left(-2\pi^2l^2n^2s_g^2\right) - 4\pi^2l^2ns_g^2A_n \quad (3)$$

$$= \frac{dA^P_{nc}}{dn}\exp\left(-\frac{\pi^2lns_c^2}{\sigma}\right) - \frac{\pi^2ls_c^2}{\sigma}A_n\,. \quad (4)$$

From equations (3) and (4), we obtain

$$\left(\frac{dA_n}{dn}\right)_{n=0} = \left(\frac{dA^P_{ng}}{dn}\right)_{n=0} \quad (5)$$

and

$$\left(\frac{dA_n}{dn}\right)_{n=0} = \left(\frac{dA^P_{nc}}{dn}\right)_{n=0} - \frac{\pi^2ls_c^2}{\sigma}A_0\,. \quad (6)$$

Since A_0 is made equal to 1 in the actual calculations, equation (6) becomes

$$\left(\frac{dA^P_{nc}}{dn}\right)_{n=0} = \left(\frac{dA_n}{dn}\right)_{n=0} + \frac{\pi^2ls_c^2}{\sigma} \quad (7)$$

$$= \left(\frac{dA_{ng}}{dn}\right)_{n=0} + \frac{\pi^2ls^2}{\sigma} \quad (8)$$

from equation (5).

Since $(dA^P_{nc}/dn)_{n=0}$ and $(dA^P_{ng}/dn)_{n=0}$ are measures of the reciprocals of the particle sizes t_c and t_g obtained on the basis of Cauchy and Gauss strain distributions respectively, it is obvious from equation (8) that t_c is very nearly equal to t_g when s_c^2 is negligibly small. For an appreciable value of s_c^2, t_c should be different from t_g and $t_g > t_c$.

Next, suppose that we are determining the strain from a study of two reflexions $00l$ and $002l$ and let A_{n1} and A_{n2} be the nth order Fourier coefficients of the two reflexions respectively. Then, again from equations (1) and (2) and noting that both A^P_{ng} and A^P_{nc} are same for the two reflexions, we have

$$\ln A_{n1} - \ln A_{n2} = 6\pi^2l^2n^2s_g^2 \quad (9)$$

$$= \pi^2(ln/\sigma)s_c^2\,. \quad (10)$$

From equations (9) and (10), we have

$$s_c^2 = 6\sigma lns_g^2 \quad (11)$$

and

$$s_c = \sqrt{6\sigma\langle ln\rangle}\,.\,s_g\,. \quad (12)$$

Thus, for ordinary values of $\sigma(\sim 0{\cdot}2)$, the ratio $s_c/s_g > 1$ and is dependent on l as well as the number of orders over which the determination has been carried out. For $n=1$ and $\sigma=0{\cdot}2$,

$$s_c/s_g = 1{\cdot}44 \text{ for 111–222 reflexions}$$
$$= 1{\cdot}55 \text{ for 200–400 reflexions}\,.$$

Actually s_c and s_g are sought to be determined at $n=0$, which is done by graphical extrapolation which practically means averaging over several orders. Hence s_c experimentally determined is approximately one and a half times s_g, and sometimes even more, as has been observed by previous authors.

Thus while the experimental results on the relation between s_c and s_g are in agreement with the theoretical predictions presented here, the relation between t_c and t_g as obtained by previous workers is in contradiction to the theoretical results obtained in course of the present study. This is because the ratio $s_c:s_g$ depends on the two strain hypotheses (*cf.* equations (9) and (10)) and is independent of experimental data but for the extrapolation of s_c and s_g to $n=0$. On the other hand, the ratio of t_c to t_g depends on the experimentally determined quantity $(dA_n/dn)_{n=0}$ which is sensitive to different experimental errors including inability to fix the proper background level and neglect of the contribution due to thermal diffuse scattering. This perhaps explains, at least to some extent, the discrepancy between theoretically derived and experimentally obtained values of the ratio $t_c:t_g$. An alternative explanation may be that, as shown by Mitra (1963), the actual strain distribution is probably neither of the Cauchy nor of the Gauss type, so that both equations (1) and (2) are incorrect, and hence the results derived from them do not agree with experimental results.

References

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