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X-ray diffraction line profile from the aggregate of distorted crystallites. II

G B MITRA and T B GHOSH*

Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700032, India

*Department of Physics, Indian Institute of Technology, Kharagpur 721 302, India

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Abstract. An expression for the fourth moment of the line profile in terms of several strain derivatives and the possibility of measuring the 'wavelength' of crystal distortions (λ) for any sinusoidally varying component of the strain are available. The experimental means for evaluating such strain derivatives in the expression for the fourth moment was earlier described. A numerical method for evaluating this wavelength and its subsequent use to determine λ in several samples of α-brass is presented here. The data used are taken from the earlier paper of the authors. An attempt has been made to interpret the values of λ and their changes with cold working and annealing in terms of lattice strain.

Keywords. Wavelength of distortion wave; strain gradient; fourth moment; X-ray diffraction profile; distorted crystallites.

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1. Introduction

Mitra (1964) had studied properties of the fourth moment of the line profile due to aggregates of distorted crystallites and derived the following expression for the fourth moment of the strain profile

$$\begin{aligned}\mu_s = &-[(\sigma_1+\sigma_2)/2\pi^3]\cdot[(3\pi\langle ee'\rangle - 2\langle e\rangle\langle e'\rangle)/d^2] \\ &-(1/4\pi^2)\cdot[(4\langle ee''\rangle + 3\langle e'^2\rangle - 4\langle e\rangle\langle e''\rangle)/d^2] \\ &+(\langle e^4\rangle - 4\langle e^3\rangle\langle e\rangle + 6\langle e^2\rangle\langle e\rangle^2 - 3\langle e\rangle^4)/d^4, \end{aligned} \tag{1}$$

where μ_s is the fourth moment due to strain, σ_1 and σ_2 are the ranges, e, e', e'' are the strain and their space derivatives, $\langle\ \rangle$ indicates the average over the crystallite and d is the interplanar spacing. We assume that e can be expressed as a sinusoidal function of the distance t in the crystallite and can be expressed as,

$$e = e_0 \sin[(2\pi/\lambda)]t, \tag{2}$$

where λ is the wavelength of the distortion wave. Mitra (1964) showed that the ratio of the range-independent second term to the range-dependent first term will be of the order of $\pi/\lambda\sigma$. This ratio which is proportional to the inverse of the wavelength can be determined by plotting μ_s against $\sigma = \sigma_1 + \sigma_2$. The resultant plot will be a straight line where the intercept with the μ_s axis will give the second term and the slope will obviously give the value of first term. Mitra and Ghosh (1987, hereafter referred to as paper I) have described the experimental methods for determining these two terms in several samples of α-brass. The contribution due to the third term was not considered because it is of the order of e^4/d^4, which is negligibly small when compared with other terms.

While the above considerations give an idea about the order of magnitude of the wavelength of the distortion waves, the exact value of λ can be obtained only by direct calculations. It is well known that dislocation movements caused by externally applied mechanical stress during cold working or thermal stresses during annealing, quenching etc obey wave equations and hence can be expressed in terms of displacements having wave nature (Love 1944; Eshelby 1949). Thus the wavelength of distortion waves is an important parameter for studies in characterization of distorted materials.

Experimental details for evaluation of the terms in the expression of fourth moment (1) were reported in paper I. It had been done for 70:30, 80:20, 90:10 wt% of Cu:Zn at different stages of cold working and annealing. The present work attempts to determine the exact wavelength of the distortion wave in the above alloys and investigate the variation, if any, in the wavelength during mechanical and thermal processes of cold working and annealing. For this purpose the ratio of the second and first terms of (1) has been numerically evaluated, taking e as a sinusoidal function of distance t.

2. Ratio in terms of wave-like strain displacements

As mentioned earlier the distortion wavelengths inside polycrystalline materials have been estimated assuming that the strain inside a crystallite can be expressed as a sinusoidal function of distance t. Thus e can be expressed as

$$e_0 \sin [(2\pi/\lambda)]t.$$

The average of e over the entire length of each crystallite can be expressed as

$$\langle e \rangle = \langle e_0 \sin (2\pi/\lambda)t \rangle$$
$$= (1/T)e_0 \int_0^T \sin [2\pi/\lambda]t \, dt,$$

where T is the average linear dimension of the crystallites. In the present treatment λ is assumed to be accommodated inside T, such that $T = n\lambda + x\lambda$, where n is an integer and x is a fraction.

Thus

$$\langle e \rangle = (e_0/2\pi)(\lambda/T)[1 - \cos 2\pi x].$$

Assuming $x \ll 1$,

$$\langle e \rangle \simeq (e_0/2T)(\lambda/T)\cdot[(2\pi x)^2/2] = e_0\cdot(\lambda/T)\cdot \pi x^2.$$

Thus,

$$\langle e \rangle = \pi e_0 \cdot (\lambda/T)\cdot x^2. \tag{3}$$

Similarly

$$\langle e' \rangle = 2\pi e_0(1/T)\cdot x^2, \tag{4}$$

$$\langle ee' \rangle = 2\pi^2 e_0^2(1/T)\cdot x^2, \tag{5}$$

$$\langle e'' \rangle = -4\pi^3\cdot e_0(1/\lambda T)\cdot x^2, \tag{6}$$

$$\langle ee'' \rangle = -2\pi^2 e_0^2(1/\lambda T)[T/\lambda - x], \tag{7}$$

$$\langle e'^2 \rangle = 2\pi^2 e_0^2(1/\lambda T)[T/\lambda + x]. \tag{8}$$

Thus

$$\begin{aligned} &3\pi\langle ee' \rangle - 2\langle e \rangle\langle e' \rangle \\ &\quad = 6\pi^3 e_0^2(1/T)\cdot x^2 - (2\pi e_0)^2(\lambda/T^2)\cdot x^2 \\ &\quad \simeq (6\pi^3 e_0^2/T)\cdot x^2 \text{ [neglecting higher power of } x\text{].} \end{aligned} \tag{9}$$

and

$$\begin{aligned} &4\langle ee'' \rangle + 3\langle e'^2 \rangle - 4\langle e \rangle\langle e'' \rangle \\ &\quad = 2(\pi e_0)^2(1/\lambda T)[7x - T/\lambda] \text{ [neglecting higher power of } x\text{].} \end{aligned} \tag{10}$$

Writing $T/\lambda = n + x$, equation (10) becomes

$$-[2(\pi e_0)^2/\lambda T]\cdot[n - 6x].$$

Hence we get,

$$\begin{aligned} \text{ratio term } (f_E) &= (\pi/2)\cdot[(4\langle ee'' \rangle + 3\langle e'^2 \rangle - 4\langle e \rangle\langle e'' \rangle)/ \\ &\qquad (3\pi\langle ee' \rangle - 2\langle e \rangle\langle e' \rangle)] \\ &= (1/6T)\cdot[(n^2 - 5nx - 6x^2)/x^2]. \end{aligned} \tag{11}$$

Assuming $n = 1$, i.e., when one full wave and a fraction of it are accommodated inside the crystallite, the above expression reduces to

$$\text{ratio term } (f_E) = -(1/6T)\cdot[(1 - 5x - 6x^2)/x^2]. \tag{12}$$

It turns out that the ratio is a function of crystallite size (T) and the fractional number x. The details of evaluation of the ratio term (f_E) for a given crystallite size were described in paper I. To find x, the function $1/6(1 - 5x - 6x^2)/x^2$ is plotted as a function of x (figure 1). For an experimentally obtained value of the product of ratio and crystallite size gives a value of the function $1/6(1 - 5x - 6x^2)/x^2$. Thus using figure 1, one can obtain the particular value of x. Again $T = n\lambda + x\lambda$, gives an idea of the wavelength of the distortion wave. In the present studies n is assumed to be equal to 1. While working out an expression for λ, the present results indicate that, probably x, the fraction of a full wave accommodated inside the crystallite, gives an idea of the extent of lattice distortion. It is apparent that x can in a way be defined as a lattice strain and therefore from the values of x one can interpret the extent of defect present in a crystallite.

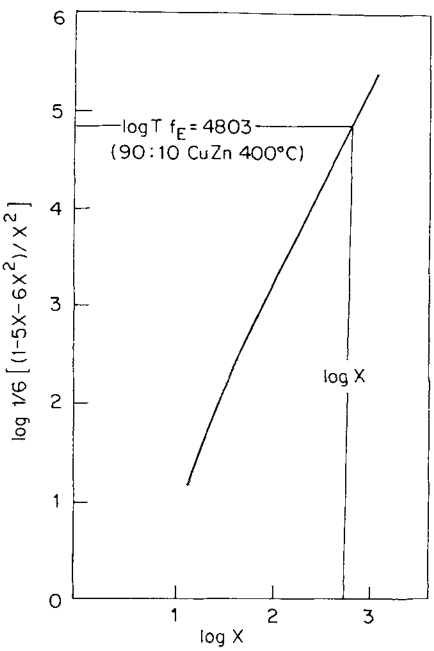

Figure 1. Plot of logarithm of the function of x for various values of logarithm of x.

In the present investigations x has been evaluated for several samples of Cu:Zn alloy. The changes of x with cold working and subsequent annealing have also been reported.

3. Results and discussion

Table 1 gives the values of crystallite size, r.m.s. strain and several strain derivatives obtained experimentally as reported in paper I. Table 2 gives the corresponding value of the ratio terms. These values have subsequently been used to find x i.e. the fraction of the full wavelength present inside the crystallite (figure 1).

Table 3 shows that as the values of crystallite size increase, x decreases. This probably indicates that for a larger crystallite size the lattice strain at the boundary of the crystallite is less. Thus the parameter x may be used to find out the extent of lattice strain at the boundary of a crystallite in a polycrystalline material.

It is apparent from (12) that as x tends to zero, the ratio (f_E) tends to infinity. This situation arises only when $T = n\lambda$, i.e. a full wavelength or an integral multiple of it is accommodated inside the crystallite. This indicates a physically improbable situation as the lattice strain in this case will be zero.

The above studies lead us to the conclusion that x is an important parameter for the studies of lattice imperfections inside the polycrystalline material. It may be noted here that the exact value of λ can only be known only when n is known. In the present investigation the value of n is assumed to be equal to 1. Further studies to evaluate the exact value of λ, and the correlation of x or λ with different types of dislocations are in progress.

Table 1. Values of r.m.s. strains and other strain gradients obtained experimentally for three different compositions of Cu:Zn at various stages of cold working and annealing.

Composition	Annealing temperature (°C)	$\langle e^2 \rangle^{1/2} \times 10^3$	$\langle ee' \rangle$ (cm^{-1})	$[4\langle ee'' \rangle + 3\langle e'^2 \rangle] \times 10^{-10}$ (cm^{-2})
	CW	8·2	6·470	−1·141
	100	8·4	4·390	−0·880
90:10	200	7·8	3·114	−0·601
Cu:Zn	300	7·2	2·079	−0·479
	400	7·0	0·462	−0·261
	CW	9·4	2·883	−1·167
	100	8·1	7·624	−1·472
80:20	200	7.4	2·883	−0·853
Cu:Zn	300	7·0	1·728	−0·514
	400	6·9	0·462	−0·209
	CW	7·2	71·6	−0·900
70:30	300	6·6	9·00	−0·219
Cu:Zn	400	6·6	8·95	−0·132

Table 2. Values of crystallite size and the corresponding values of f_E obtained experimentally for different compositions of Cu:Zn at various stages of cold working and annealing.

Composition	Annealing temperature (°C)	Crystallite size (T) (Å)	Ratio (f_E) $\times 10^{-6}$ (cm^{-1})
	CW	338	293·9
	100	779	334·1
90:10	200	1126	321·7
Cu:Zn	300	1188	384·0
	400	6755	941·0
	CW	316	674·6
	100	349	321·8
80:20	200	1013	493·12
Cu:Zn	300	2026	495·7
	400	6755	753·9
	CW	181	21·47
70:30	300	3377	40·55
Cu:Zn	400	5066	24·58

Note: ratio (f_E) is obtained from table 1.

Table 3. Crystallite size, r.m.s. strain and x as obtained for different compositions of Cu:Zn at different stages of annealing and cold working.

Composition	Temperature (°C)	Crystallite size (T) Å	r.m.s. strain $\langle e^2 \rangle^{1/2} \times 10^3$	Fraction of distortion wave-length $(x) \times 10^3$
	CW	338	8·2	12·00
	100	779	8·4	7·94
90:10	200	1126	7·8	7·08
Cu:Zn	300	1188	7·2	5·62
	400	6755	7·0	1·58
	CW	316	9·4	8·91
	100	349	8·1	11·00
80:20	200	1013	7·4	5·62
Cu:Zn	300	2026	7·0	3·98
	400	6755	6·9	1·78
	CW	181	71·6	63·1
70:30	300	3377	9·0	11·00
Cu:Zn	400	5066	9·0	11·00

Note: x is evaluated from figure 1.

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