Nature of Mean Square Strain

Hidewo TAKAHASHI

(Received October 7, 1985)

Faculty of Education
Kagoshima University
Kagoshima 890, Japan

Abstract

Nature of mean square strain obtained by X-ray line profile analysis is discussed. The so-called mean square strain is not mean square strain in true meanings but the variance of the strain. Strain function discussed by Turunen, de Keijser, Delhez and van der Pers (J. Appl. Cryst. (1983). **16**, 172) is shown not to be suitable for strain analysis by line profile analysis.

1. Introduction

Strain determination of cold-work metal by line profile analysis of X-ray reflection was discussed more than about thirty years ago. The study was classified into two categories, one was dependent upon theoretical study of Eastabrook and Wilson (1952) and the other was dependent upon experimental study of Warren school. Many investigators arranged experimental data by Warren's method, socalled Warren and Averbach method, and interpreted the results by the theory of Eastabrook and Wilson (1952). The theory of Eastabrook and Wilson is very acceptable to physicists, but has a defect in statistical treatment of strain function. Because of this, many questions arose in the line profile analysis. Williamson and Smallman (1954) discussed that since the line profile should be of the same form with strain distribution function and the observed line profiles were of Cauchy type and hence the strain distribution must be of Cauchy type, then mean square strain would diverge. They proposed tricky mathematical devices for avoiding the difficulty. The author (Takahashi (1969)) succeeded to show that the line profile of Cauchy type could be obtained from Gaussian distribution of strain and that Warren's experimental results could be interpreted by two parameters. The same parameters were obtained by Adler and Houska (1979).

Recently, Turunen, de Keijser, Delhez and van der Pers (1983) published an article discussing the strain function along line of Eastabrook and Wilson (1952). The author was surprised when he read their article and found very small quantities for describing their strain function. The very small quantities with order from 10^{-10} to 10^{-63} may not have any physical meanings in describing strain function, because the X-ray diffracted intensity is macroscopic observable quantity. The small quantitites must be necessary for convergence of their strain function. The author's judgement is that the small quantities are the proof of the bankrupt of their theory. The causes driving them to the strange conclusions aremainly the following three. At first, their understanding of strain function is wrong. Secondly, they do not understand nature of X-ray reflection by polycrystalline materials. At last and essentially their mathematical faculty is extremely low to discuss this problem.

In this article, the author clarifies the meanings of mean square strain and discusses the theory of Turunen *et al.*

2. Nature of strain function

Let us examine X-ray reflection from a column perpendicular to the reflecting planes. The column length is assumed to be L_0, and the spacing of the reflecting planes to be d. The column is also assumed to be parallel to c-axis, that is, the diffraction index is $00l$, and the axis length to be c. When local strain, which is the ratio of the lengths before and after the stress is added at the position between z and $z+dz$, is denoted by $e(z)$. Turunen *et al.* introduced a function $E(\zeta)=e(z-z_0)$, where $\zeta=z-z_0$. They developed $E(\zeta)$ by the following form,

$$E(\zeta)=e(z_0)+\sum_{n=1}^{\infty}\frac{e^{(n)}(z_0)}{n!}\zeta^n \tag{1}$$

The author points out that their definition of $E(\zeta)$ is wrong, since $E(\zeta)$ should be developed by the following form,

$$E(\zeta)=e(0)+\sum_{n=1}^{\infty}\frac{e^{(n)}(0)}{n!}\zeta^n \tag{2}$$

if $\zeta=z-z_0$. We can judge from eq. (1) that $E(\zeta)$ is equal to $e(z)$ developed around z_0.

$$\begin{aligned} e(z)&=e(z_0+\zeta)\\ &=e(z_0)+\sum_{n=1}^{\infty}\frac{e^{(n)}(z_0)}{n!}\zeta^n\\ &=E(\zeta). \end{aligned}$$

The author points out that the degree of their mistake to develop $E(\zeta)$ by eq. (1) is lower than high school student level. Why can $E(\zeta)$ be developed around z_0 in the case of $\zeta=z-z_0$? When $\zeta=0$, then $z=z_0$.

The average value of $E(\zeta)$ for column length L is denoted by $\varepsilon(L)$, and is given by

$$\varepsilon(L)=\frac{1}{L_0-L}\int_{\frac{L}{2}}^{L_0-\frac{L}{2}}E(\zeta)d\zeta$$

$$=e(z_0)+\sum_{n=1}^{\infty}\frac{e^{(2n)}(z_0)}{(2n+1)!2^{2n}}L^{2n}. \tag{4}$$

The average value $\varepsilon(L)$ depends on the position z_0, so that $\varepsilon(L)$ should be rewritten by $\varepsilon(L, z_0)$. The average of mean square of $\varepsilon(L, z_0)$ should be expressed by

$$\langle\varepsilon(L)^2\rangle=\frac{1}{L_0-L}\int_{\frac{L}{2}}^{L_0-\frac{L}{2}}\varepsilon(L, z_0)^2dz_0$$

$$=\sum_{n=0}^{\infty}C_{2n}L^{2n}. \tag{5}$$

The average value $\langle\varepsilon(L)^2\rangle$ is not a function of z or z_0.

Those who regard the coefficients in eq. (5) are functions of position z or z_0 can not understand the meanings of the average. The average is to be done over position z or z_0. Hence the partial integrations of the coefficients as functions of z are nonsense. Even the partial integrations are possible, their boundary condition setting is wrong, since the range of the integration is $L/2 \leq z \leq L_0-L/2$.

The average value $\langle\varepsilon(L)^2\rangle$ as a function of L is a rapidly decreasing function from Turunen *et al.*'s experimental results and interpretation. But local strain $e(z)$ should be very slowly variable function in a column. In addition, $\langle\varepsilon(L, z_0)\rangle$ should converge to e_0, the strain of the column, when L converge to L_0.

3. Nature of distortion coefficients

The experimental results of Turunen *et al.* were quite different from those deduced from true mean square strain discussed in the preceding section. They misunderstood that so-called mean square strain obtained from the line profile analysis was really mean square strain and that the line profile consisted of reflection of a single column.

If Turunen *et al.* carefully read articles of Eastarook and Wilson (1952) and the author's (1969), they should find that the so-called mean square strain was not mean square strain but the variance of the strain. Their experimental results were obtained from cold-rolled aluminium sheet. Local strain $e(z)$ may be nearly constant and equal to the strain of the column. Then, true mean square strain becomes nearly constant and converges to e_0^2. The average strain is observed by the shift of center of gravity of the line profile from the Bragg position of unstressed materials. The so-called mean square strain is square of strain minus e_0 in case of single column reflection.

Turunen *et al.*, even Adler and Houska (1979), interpreted Fourier coefficients of the line profile assuming that the line profile was generated from reflection of a single column. By taking account of the experimental condition of generating the line profile, this assumption is far away from reality. Adler and Houska's interpretation of distortion coefficients, which are the same as the author's ones, is unreasonably strange. Adler and Houska considered that there was a distribution of uniform strain in a column. We can not imagine varying uniform strain in a column. If we change the interpretation of the uniform strain in a column to the average strain of the column and the distribution of the strain in the column to the distribution of columns with the average strain in reflecting columns, we can understand reasonably the coefficients. This interpretation was already made in the author's article. Hence, the distortion coefficients consist of two variances, one is the variance of the average strain in reflection columns and the other is the variance of inhomogeneous or local strain in a column.

References

Adler, T. and Houska, C.R. (1979). J. Appl. Phys. **50**, 3282.
Eastabrook, J.N. and Wilson, A.J.C. (1952). Proc. Phys. Soc. London. **B, 65**, 67.
Takahashi, H. (1969). J. Phys. Soc. Japan. **27**, 708.
Turunen, M.J., de Keijser, Th. H., Delhez, R. and van der Pers, N.M. (1983). J. Appl. Cryst. **16**, 176.
Williamson, G.K. and Smallman, R.E. (1954). Acta Cryst. **7**, 574