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ANALYSIS OF DISPLACEMENT AND BROADENING OF X-RAY DIFFRACTION LINES CAUSED BY SURFACE STRESS GRADIENT: COMPUTER SIMULATION AND MEASUREMENT

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Abstract. Some problems arise in the case of residual stresses measurements by X- ray diffraction technique when analyzed stress state is characterized by strong gradient on the surface of a material. These problems include the fact that linear dependence of the diffraction angle $\theta_{\varphi,\psi}=f(\sin^2\psi)$ becomes nonlinear. Besides, there is broadening of diffraction line caused by surface stress gradient. If the first problem makes difficulty to calculate the value of mechanical stresses, the second provides an opportunity to find the relationship between the diffraction line width and stress gradient parameters. Analysis of nonlinear displacement with broadening of diffraction line and development of methodology of stress determination with strong gradient is the objective of this paper.

1. INTRODUCTION

Modern technologies of material surface treatment like laser or ion beam technologies produce high surface residual stresses characterized by strong gradients of stress distribution in depth of a treated material. X-ray tensometry [1,2] well known as the experimental method of traditional stress measurements can be applied to analysis of stress gradients too [2,3]. Analysis of non-linearity of experimental curve $\theta_{\varphi,\psi}$ *versus* $\sin^2\psi$, that is the base of X-ray diffraction method of stress measurements, allows evaluate the parameters of stress gradient, however, this method has difficulties because of this non-linearity is often invisible experimentally. Other difficulty is that the absence of criterions of existence of stress gradients reduces sensitivity of direct mathematical solution of strain equations to obtain analytically stress gradient parameters [4].

In this paper computer simulation is used both to obtain the criterions of existence of surface stress gradients and to resolve the problem of experimental determination of stress gradients by X-ray diffraction technique. Fourier analysis, widely used in different fields of modern physics, can be applied to study the broadening of diffraction profile caused by the presence of surface stress gradient. The function responsible for diffraction line broadening depends on X-ray penetration into the analyzed material and the magnitude of stress gradient parameters. Extracting this function (distortion function) allows use it in the determination of stress distribution near the surface of a material.

2. METHODOLOGY OF COMPUTER SIMULATION OF DIFFRACTION PROFILE

Methodology of computer simulation is based on consideration of contribution of all subsurface layers of material for intensity and position of diffraction line [5]. Taking into account an attenuation of X-rays into material and path for incident and diffracted beams it is possible to obtain the intensity

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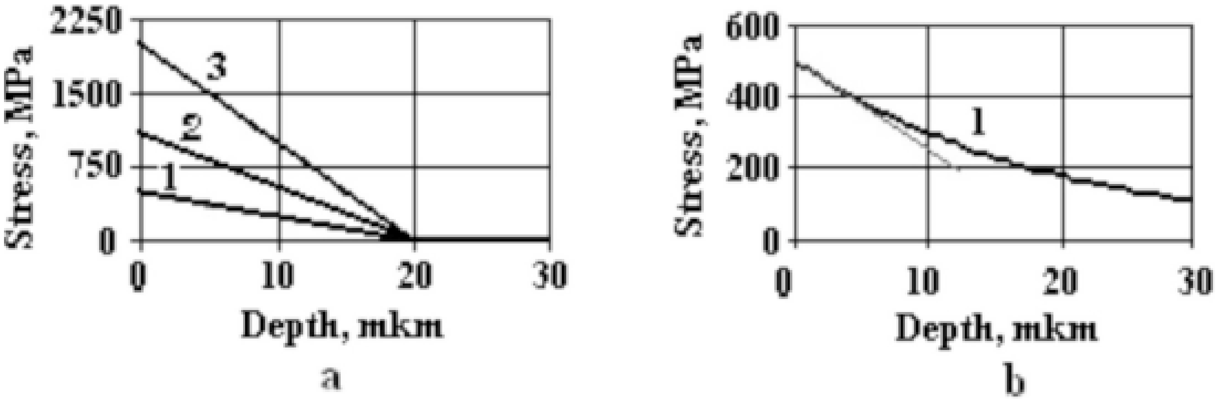

Fig. 1. Linear (a) and exponential (b) stress distributions with different gradients: 1(a, b) – 25 MPa/μm; 2 – 50 MPa/μm; 3 – 100 MPa/μm.

reflected by any subsurface layer. The following equations describe this process:

$$I(z) = I_0 e^{-\mu z}, \tag{1}$$

$$z = t\left[\frac{1}{\cos(\psi + 90 - \theta)} + \frac{1}{\cos(\psi - 90 + \theta)}\right], \tag{2}$$

$$I_{dif} = aI_0 e^{-\mu t\left[\frac{1}{\cos(\psi+90-\theta)}+\frac{1}{\cos(\psi-90+\theta)}\right]}. \tag{3}$$

Here z is the path of passing for incident and diffracted beams into material, t is the depth of the surface layer penetrated by X-ray beam, ψ is the angle between the normal to the material surface and normal to the diffraction plane, θ is the diffraction angle, μ is the absorption coefficient of the analyzed material and α is a coefficient of proportionality for intensity of diffracted beam I_{dif}.

Eq. (3) can be interpreted as contribution of each subsurface layer for total intensity of diffraction line. Angular position of this part of diffraction intensity can be determined by the value of interplanar distance that, on the other hand, depends on the stress distribution $\sigma(t)$. In the paper we used linear and exponential stress distributions expressed as:

$$\sigma(t) = \sigma_0 + kt, \tag{4a}$$

$$\sigma(t) = \sigma_0 e^{-kt}, \tag{4b}$$

where σ_0 is the stress value on the surface of material and k is the value of stress gradient. Eqs. (4a) and (4b) allow obtain the magnitude of strain for any layer t and for any direction ψ. From the theory of elasticity, the strain in arbitrary $\varepsilon_{\varphi\psi}$ direction can be expressed as:

$$\varepsilon_{\varphi\psi} = \frac{1+\nu}{E}\sigma(t)\sin^2\psi - \frac{\nu}{E}(\sigma_1 + \sigma_2). \tag{5}$$

Here ν and E are the material elastic constants, σ_1 and σ_2 are the principal stresses. For one-dimensional stress state $\sigma_1 = \sigma(t)$ and $\sigma_2 = 0$. For this case, Eq. (5) is transformed as:

$$\varepsilon_{\psi} = \frac{\sigma(t)}{E}\left[(1+\nu)\sin^2\psi - \nu\right]. \tag{6}$$

Eq. (6) can be expressed in diffraction terms too. Using Bragg's law it can be written as:

$$\varepsilon_{\psi} = \frac{d_{\psi} - d_0}{d_0} = -(\theta_{\psi} - \theta_0)\cot\theta, \tag{7}$$

where d_0, d_{ψ}, θ_0, θ_{ψ} are the interplanar distances and diffraction angles for unstressed and analyzed material, respectively. Equating and simplifying Eqs. (6) and (7), we can obtain the formula for diffraction angle distribution as a function of depth t and polar angle ψ:

$$\theta_{\psi} = \theta_0 - \frac{\sigma(t)}{E}\left[\sin^2\psi - \nu\cos^2\psi\right]\cos\theta_0 \tag{8}$$

Eq. (8) characterizes the angle position of individual diffraction lines reflected by any subsurface layer being into depth t. It depends on stress distribution $\sigma(t)$ and stress gradient k. In this paper there were analyzed the following stress distributions:

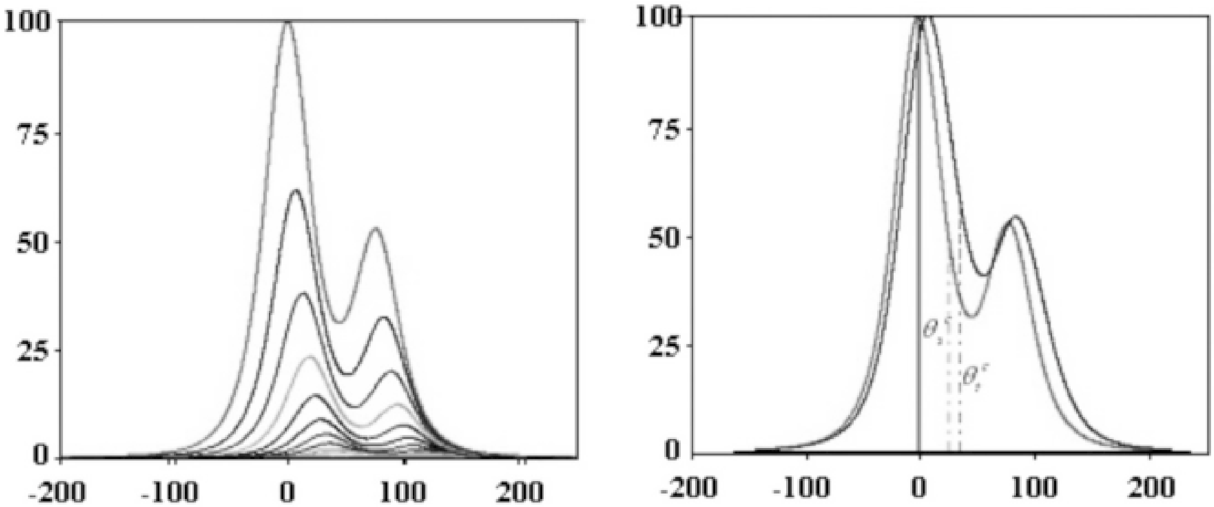

Fig. 2. Simulation of diffraction profile for linear σ(*t*) = 500 - 25*t* and exponential σ(*t*) = 500$e^{-0.05t}$ stress distributions: a - profiles formed by individual layers; b - standard profile (red) and total profile (blue) formed by all layers.

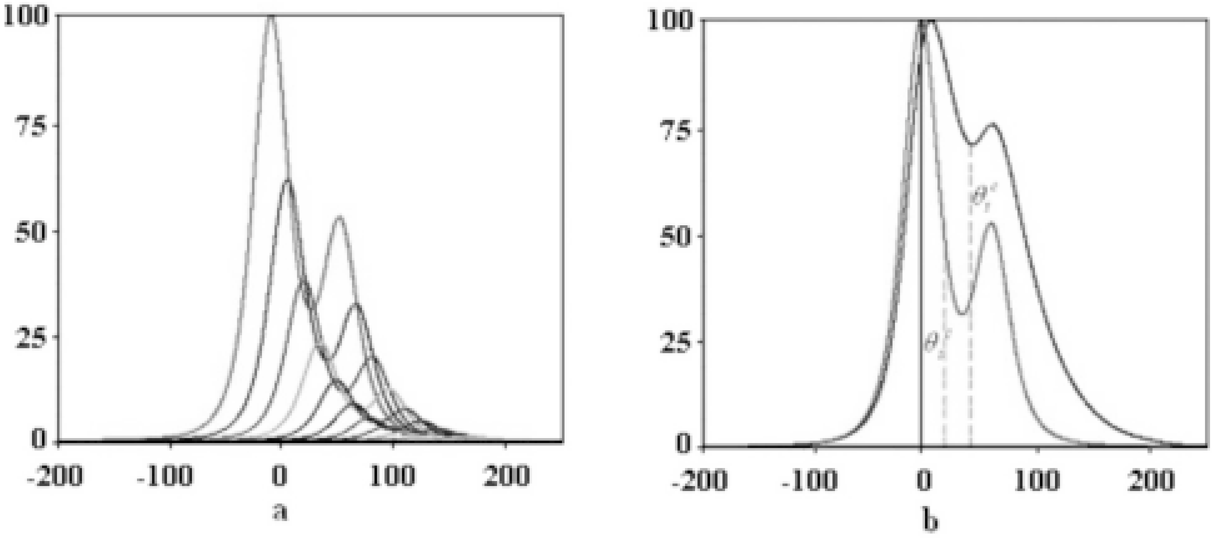

Fig. 3. Simulation of diffraction profile for linear stress distribution σ(*t*) = 2000 - 100*t*; a - profiles formed by individual layers; b - standard profile (red) and total profile (blue) formed by all layers.

$$\sigma(t) = 500 - 25t, \quad (9a)$$

$$\sigma(t) = 500e^{-0.05t}, \quad (9b)$$

$$\sigma(t) = 1000 - 50t, \quad (9c)$$

$$\sigma(t) = 2000 - 100t, \quad (9d)$$

Stress gradients for used functions were varied from *k* = 25 MPa/μm for function (9a) to *k* = 100 MPa/μm for (9d). Fig. 1 illustrates these stress distributions.

Computer simulation of diffraction profile is based on the using of equations (3) and (8) which characterize the intensity and angle position of individual diffraction lines from each subsurface layer into depth *t*. The sum of these individual profiles forms the total diffraction line. The thickness of each individual layer for our simulation was 0.1μm and simulation process was finished when the layer intensity become less then the 1% from initial in-

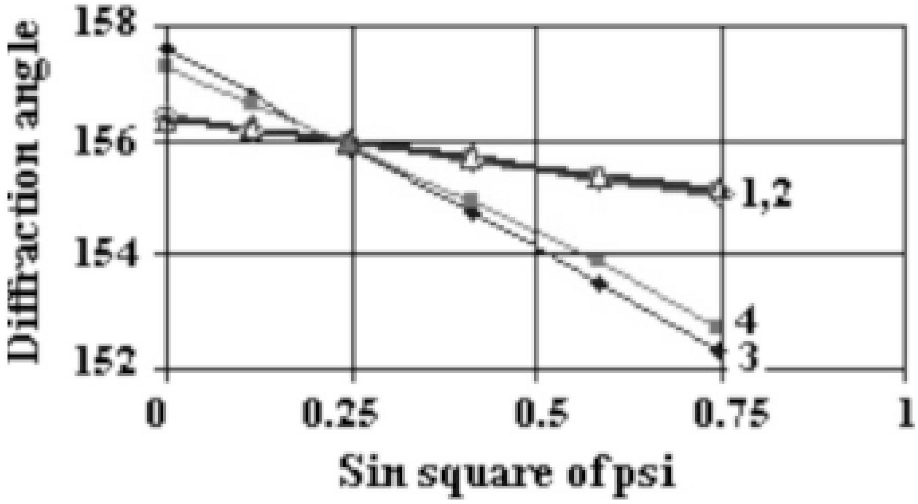

Fig. 4. Simulated plots 2θ versus $\sin^2\psi$ for stresses without gradient (lines 1, 3) and with gradient (curves 2, 4). Graphs (1, 2) and (3, 4) correspond to the cases $\sigma(t) = 500 - 25t$ and $\sigma(t) = 2000 - 100t$, respectively.

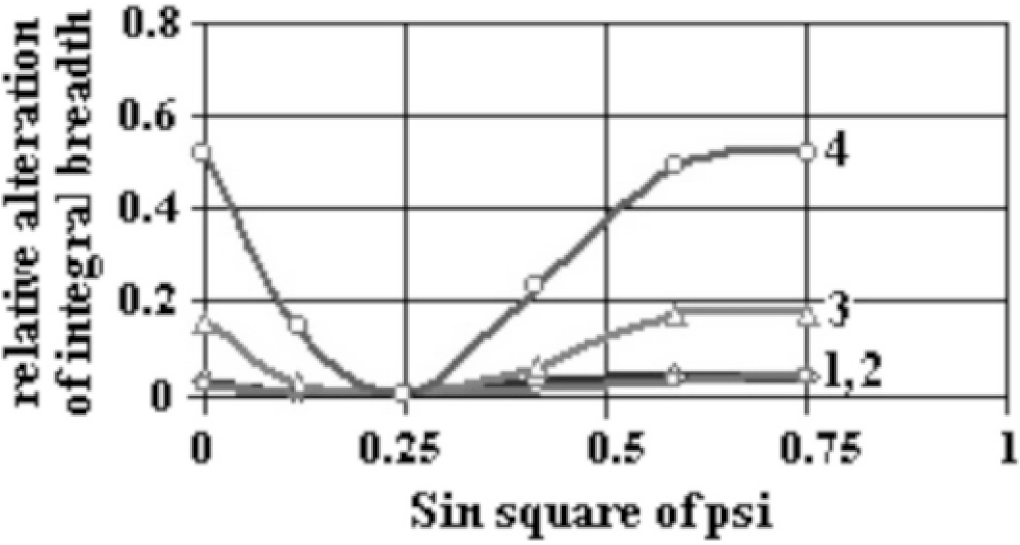

Fig. 5. Integral breadth ΔB/B versus $\sin^2\psi$ for different stress distributions: 1) $\sigma(t) = 500 - 25t$; 2) $\sigma(t) = 500e^{-0.0515t}$; 3) $\sigma(t) = 1000 - 50t$; 4) $\sigma(t) = 2000 - 100t$.

tensity. Approximated function used for individual profile was the Cauchy function. The breadth and doublet distance $K_{\alpha1-\alpha2}$ of standard profile were the same as in the case of stress measurements in steel with using of Cr-K_α radiation and (211) indexes.

Figs. 2 and 3 show simulation process and the form of diffraction profiles for stress distributions with stress gradients k = 25 MPa/μm (Fig. 2) and k = 100 MPa/μm (Fig. 3).

Figs. 2 and 3 show that stress gradients cause alterations of position and form of diffraction lines proportional to the value of stress gradient k.

3. RESULTS AND DISCUSSION

3.1. Analysis of displacement of a diffraction line

Analysis of displacement of diffraction line by computer simulation duplicates the X-ray diffraction method of stress measurements well known as "$\sin^2\psi$-method". Simulation of this method is based on the using of equation (8) and processing of obtained dependency of diffraction angle $2\theta_{\varphi,\psi}$ *versus* $\sin^2\psi$. As it was mentioned above, the position and form of simulated profiles were the same as

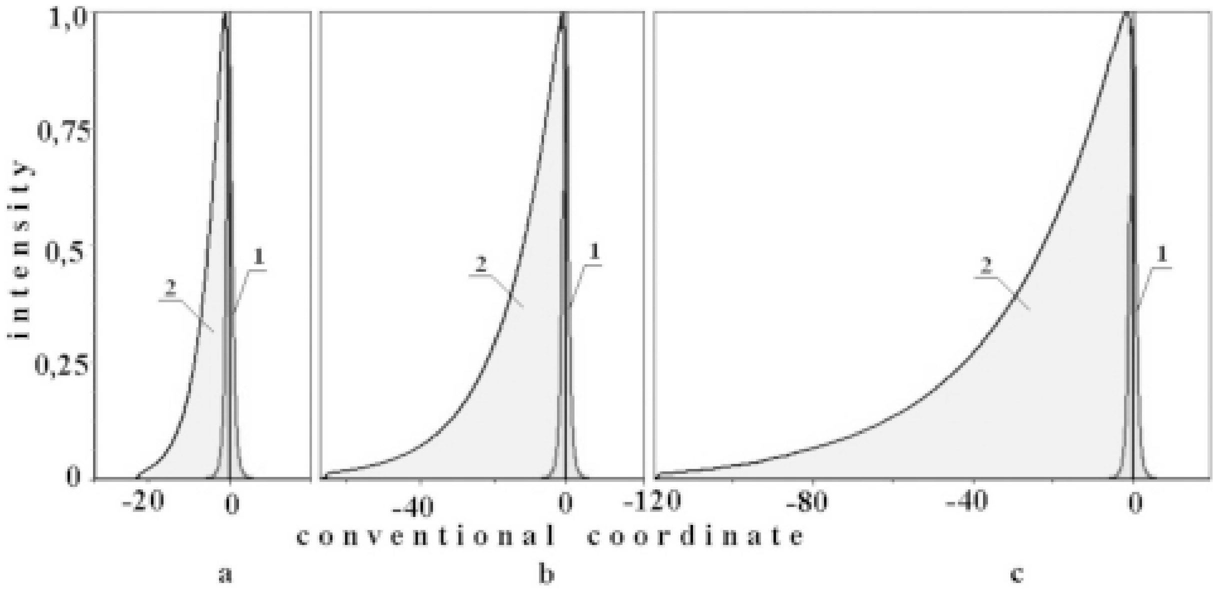

Fig. 6. Simulation of diffraction profile (2) with sharp standard function $g(x)$ (1): a) $\sigma(t) = 500 - 25t$; b) $\sigma(t) = 1000 - 50t$; c) $\sigma(t) = 2000 - 100t$.

for stress measurements in steel with Cr-K_α radiation and (211) reflections. The dependences *2*θ *versus sin*$^2\psi$ obtained by the computer simulation are presented in Fig. 4.

It can be seen that the nonlinear character of these dependences 2θ versus $\sin^2\psi$ is slightly visible, especially in the case of small gradient.

3.2. Analysis of broadening of a diffraction line

Analysis of diffraction line broadening is based on the calculation of integral breadth B that is defined as integral intensity divided on maximal intensity of diffraction peak. Fig. 5 shows relative alterations of integral breadth $\Delta B/B$ in function of $\sin^2\psi$ for different stress gradients. Graphs 1, 2 correspond to stress gradient k = 25 MPa/μm and graphs 3, 4 show behavior of $\Delta B/B$ for k = 50 MPa/μm and k = 100 MPa/μm, respectively.

Analysis of the graphs in Figs. 4 and 5 leads to the following conclusions.

1. The non-linearity of the dependence 2θ *versus* $\sin^2\psi$ is not seen clearly, but the stress gradient changes the average inclination of the lines (lines 2 and 4 in Fig. 4).

2. The alterations of the integral breadth shown in Fig. 5 are significantly larger than the displacements of the profiles shown in Fig. 4. For example, strong gradient k = 100 MPa/μm (line 4 in Fig. 5) increases the breadth of diffraction line more than 50%.

On the basis of these conclusions it can be proposed two ways to resolve the problem of measurement of stresses, characterized by strong gradient. The first way which can be applied for practical using includes the diffraction angle measurements 2θ *versus* $\sin^2\psi$ completed with the measurements of the integral breadths. The value of the integral breadth can be used to determine the gradient parameter k described the stress distribution function and to make correction of previous stress values measured by "$\sin^2\psi$–method".

Other way includes detailed analysis of diffraction line broadening caused by stress gradient. It is based on the concepts of convolution and deconvolution of Fourier transformation. In accordance with Fourier analysis the experimental diffraction line $h(x)$ can be presented as convolution of standard function $g(x)$ and distortion function $f(x)$. In the case of diffraction line broadening by stress gradient distortion function $f(x)$ depends on attenuation of X-ray beam into material and stress distribution $\sigma(t)$.

Methodology of computer simulation of X-ray diffraction profile presented in this paper allows identify the distortion function $f(x)$ responsible for this kind of diffraction line broadening. Really, convolution of any function $f(x)$ with delta-function does not change the function $f(x)$. Therefore, diffraction profile simulated with very sharp instrumental profile $g(x)$ has to form the function quasi-equal to distortion function $f(x)$. Fig. 6 demonstrates simulation of diffraction profiles with $g(x)$ like delta-function. It can be seen that simulated profile approaches to the pure distortion function $f(x)$ and the breadth of this function is proportional to the value of stress gradient k.

The form of distortion function $f(x)$ helps to find its analytical version by the following way. Using stress distribution function $\sigma(t)$ it is necessary to find first its inverse function $t=f(\sigma)$. Then the thickness t in attenuation function $I(t) = I_0 e^{-\mu t}$ can be substituted by the above inverse part of distribution function $\sigma(t)$. Using this procedure we can obtain $I(\sigma)$and then $I(\theta)$. This last substitution of σ by θ can be made by the early applied equation

$$\theta_\psi = \theta_0 - \frac{\sigma(t)}{E}\left[\sin^2\psi - \nu\cos^2\psi\right]\cos\theta_0.$$

The function $I(\theta)$ determined by this method is the distortion function which causes the broadening of a diffraction line.

4. CONCLUSION

We have analyzed the displacement and broadening of diffraction line caused by stress gradient. Software used in this paper allows not only to investigate the influence of stress gradient on position and form of diffraction profiles but also makes it possible to reproduce the distortion function which is responsible for this type of diffraction line broadening. Information about this function gives possibility to resolve the problem of nondestructive determination of distribution of residual stresses in the depth of a material.

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