46th International Scientific Conference EXPERIMENTAL STRESS ANALYSIS 2008
Department of Mechanics of Materials, VŠB - Technical University of Ostrava
June 2 - 5 2008, Horní Bečva, Czech Republic

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MICROSTRESSES AND X-RAY DIFFRACTION

MIKRONAPĚTÍ A RENTGENOVÁ DIFRAKCE

Abstract

Impacts of microscopic and macroscopic residual stresses on X-ray diffraction profiles are briefly reviewed. Depth distributions of residual stresses in a shot-peened steel sample obtained by X-ray diffraction are presented.

Abstrakt

Příspěvek popisuje vliv mikroskopických a makroskopických napětí na profily rentgenových difrakčních linií. Jsou uvedeny hloubkové průběhy zbytkových napětí v balotinované oceli, které byly získány pomocí rentgenové difrakce.

1 INTRODUCTION

Majority of engineering materials has a polycrystalline structure formed by a large quantity of randomly oriented crystal grains. Different orientation of neighbouring grains, anisotropy of elastic constants, yield strength, and material strengthening are the factors that result in different deformation of individual grains. Uneven deformation in different grains leads to generation of microstresses which are in equilibrium within microscopically small volumes of material, comparable with the grain sizes. The macrostresses are in equilibrium over the whole sample.

2 STRAIN AND STRESS

The interplanar lattice distance d_{hkl} could be computed by Bragg's law ($2d_{hkl}\sin\theta = n\lambda$) from diffraction angle θ which is measured. Differentiation of Bragg's law leads to a relation between strain of diffraction planes e_{hkl} and the diffraction angle θ:

$$e = \frac{d - d_0}{d_0} = -\Delta\theta \cot\theta_0, \tag{1}$$

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where d_0 denotes the interplanar lattice spacing in the non-deformed material. Therefore, it should be emphasized that by X-ray diffraction only elastic strains are measured. Elastic constants have to be used for stress determination. Monocrystalline elastic constants are anisotropic. For example, Young modulus E of ferrite monocrystal for crystallographic planes (*111*) is 273 GPa and 125 GPa for (*100*) planes [1]. X-ray diffraction, apart from other macroscopic methods of residual stress determination, distinguishes particular crystallographic directions. Moreover, grains in polycrystalline material are influenced by each other and, hence, some special grain-interaction models should be used [2].

2.1 Classification of stresses

When external forces and moments are absent, stresses present in the sample are called residual stresses. Three additive kinds of residual stresses in a polycrystalline material are distinguished according to the length scales (Fig 1):

$$\sigma = \sigma_I + \sigma_{II} + \sigma_{III}, \tag{2}$$

where:

σ - local stress,

σ_I - the average of the residual stresses over many grains,

σ_{II} - the difference between the average of the residual stresses over a particular grain and σ_I,

σ_{III} - the deviation of a local stress σ in a particular grain from the average stress in the grain.

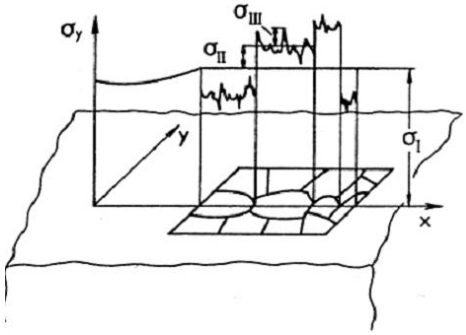

Fig. 1 The classification of stresses [3].

In the present contribution, only macroscopic residual stresses σ_I and microscopic residual stresses σ_{II} are considered.

2.2 The impact of strains on X-ray diffraction profiles

The Fig. 2 depicts diffraction profiles that are influenced by existing strains in the irradiated volume. For simplicity only three peaks from three different grains are taken into account (in reality there are thousands of grains); each peak has the width that corresponds to instrumental broadening. The "sum peak" denotes plain summation of intensities from the three particular grains. Whereas macroscopic stresses lead to a peak shift to larges diffractions angles for compressive strains (Fig. 2b), the presence of non-oriented microscopic stresses causes diffraction profile broadening (Fig. 2c).

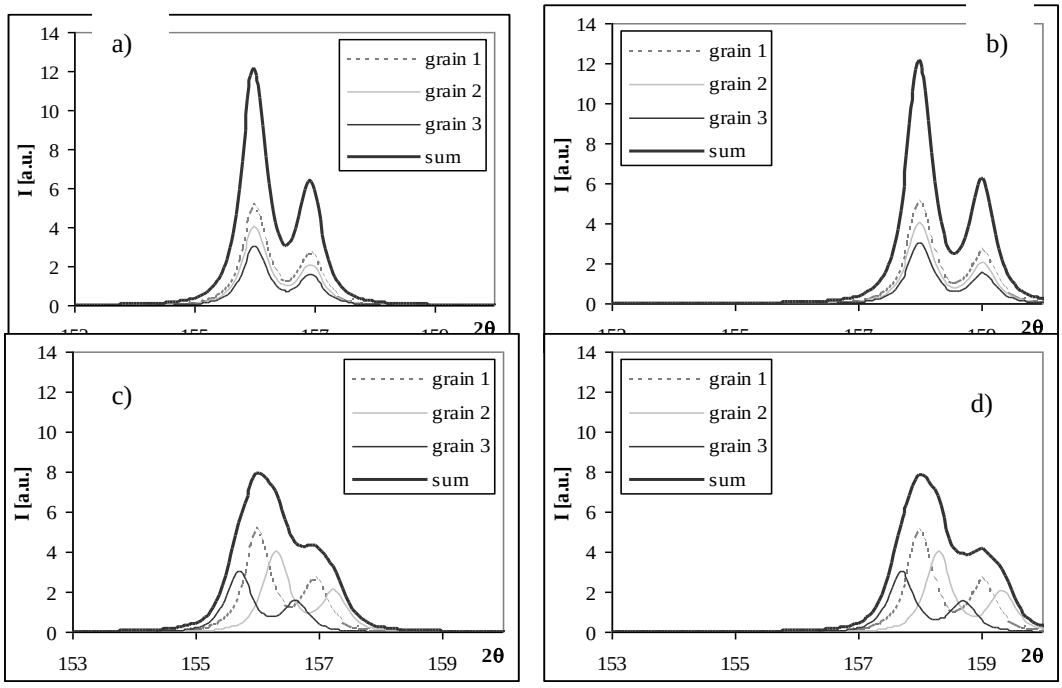

Fig. 2 The impact of stresses on X-ray diffraction peak. a) no stress, b) only macrostress, c) only microstress, d) both macro and microstress.

3 DETERMINATION OF MICROSTRAINS

It has been shown that microstrains cause broadening of diffraction peaks. The width of a diffraction peak is most often described by one of following two breadth parameters: integral breadth β or full width at half maximum *FWHM*. Both the peak parameters could be related to $\Delta\theta$ from equation (1) and then it would be transformed into [4]

$$e = \frac{1}{4}\beta \cot\theta_0 . \tag{3}$$

Therefore, the microstrains can be determined from the knowledge of breadth β and position of diffraction angle θ_0. Nevertheless, the situation is not so simple in a real material because there exist additional sources of diffraction profile broadening. Small crystallite size is another frequently occurring reason for broadening. Several methods are used to separate the influence of microstrains and crystallite size. The majority of them is based on a dependence of broadening on diffraction angle and uses several diffraction lines [5]. Other methods analyze the shape of diffraction peaks and are able to separate the broadening from crystallite size and from microstrains using one line only [6].

4 RESULTS AND DISCUSSION

The microstrains were determined in a shot-peened steel sample by single line Voigt function method [6]. The microstrains e were converted to microstresses σ^{micro} using Hooke's law ($\sigma = e\,E$) where the Young modulus 216 GPa was used. The $\sin^2\psi$ method was chosen for macroscopic residual strains determination [3]. X-ray elastic constants $½s_2 = 5.95\cdot10^{-6}$ MPa^{-1}, $-s_1 = 1.325\cdot10^{-6}$ MPa^{-1} were used in stress calculations. Since the X-ray diffraction is a surface method (the depth of studied layer is approximately several μm), electro-chemical polishing should be applied in order to remove the surface layers and study the depth of material. The Fig. 3 illustrates the depth profiles of

micro and macro stresses for two samples C11 and C13 of corrosion resistant steel. Intensity of shot peening in the case of sample C11 was lower than for C13.

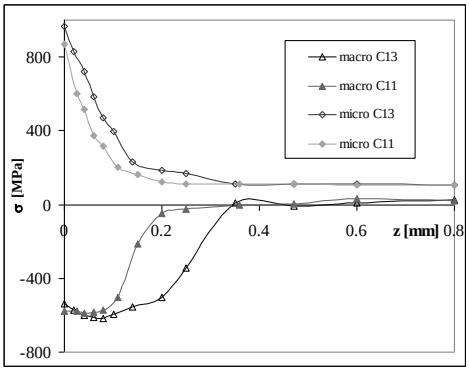

Fig. 3 The depth profiles of micro and macro stresses for samples C11 and C13 shot-peened with different intensities.

The microstresses are non-zero also in the depths which were not affected by shot-peaning which may be caused by the state of the material prior to the shot-peening process. There is a relatively big difference of macroscopic stresses on intensity of shot-peening. The surface values of crystallite size and macrostress are approximately the same for both intensities of blasting. Differences are observed primarily in the specific depth interval – from 0.15 to 0.35 mm.

5 CONCLUSIONS

The X-ray diffraction is a useful experimental technique which enables to estimate the microscopic and macroscopic stresses by a non-destructive procedure.

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ACKNOWLEDGEMENT:

The research was supported by the project No: 106/07/0805 of the Czech Science Foundation.

Reviewer: prof. MSc. Pavel MACURA, DrSc., VŠB - Technical University of Ostrava