Study by Numerical Simulation of the Influence of Surface Roughness on X-Ray Stress Measurements

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Abstract

X-ray diffraction technique is well known and well established technique applied for residual stress measurements. It is not destructive method and it is able to perform stress measurements with high accuracy and confidence. Advantages of this method stimulate its widespread use for the control of residual stresses arising in materials after various thermo mechanical treatments, after lamination, stamping and other traditional and modern technologies that are used in the manufacture and production of industrial parts and components. Several factors such as grain size, texture and surface roughness can affect the precision and accuracy of stress measurements by X-ray diffraction method. One of these factors poorly studied in the literature, is the roughness that can modify the stress distribution in the surface layer of the analyzed material, to change the actual stress value measured by X-ray diffraction method.

In this paper it was studied the influence of surface roughness on the stress measurements by X-ray diffraction technique. For this purpose it was used simulation of experimental measurements by composition of diffraction profile by the surface with different parameters of surface roughness. Database for this simulation was obtained by numerical study of surface stress distribution made by finite element method.

1 Introduction

One of the most important elements of surface topography of materials is surface roughness that is produced during machining processes like grinding, polishing etc. Surface roughness influences significantly on friction and wear characteristics of materials, affects on corrosion and fatigue resistance, changes physical properties of surface such as light reflection, heat transmission and others.

Parts or solids loaded by external forces show in homogeneous stress distribution caused by surface roughness. This stress inhomogeneity is characterized by decrease of stress value at the peak of the roughness profile and stress concentration on the bottom of the valley. It is well known that stress concentration caused by surface roughness during loading can influence significantly on mechanical behavior of material, changing, for example, its fatigue resistance [1,2], resistance to corrosion attack [3]. Inhomogeneous stress state caused by surface roughness creates also difficulties of interpretation of experimental stress measurements obtained by X-ray diffraction method [4,5].

Study of influence of surface roughness on stress measurements by X-ray diffraction technique in the present paper was achieved by simulation of X-ray diffraction stress measurements where diffraction line was composed by numerical calculations.

Information required for this procedure was obtained by 3D mapping of inhomogeneous stress distribution made by finite element method (FEM) during simulation of tensile loading applied to rectangular specimen with certain surface roughness. Carbon steel AISI 1070 with yield stress 400MPa was chosen as material of simulation.

2 Methodology

Stress distribution on the rough surface of specimen loaded by uniaxial tension was analyzed by finite element method. Simulation of mechanical behavior of steel specimen during tensile loading and 3D mapping of stress distribution on rough surface by FEM was made with using of software ANSYS®version 14.5. It was used three-dimensional model that permits to avoid some assumptions, such as plane stress hypothesis that might affect the calculation results. The scheme of mesh and loading direction of specimen is shown in Fig.1.

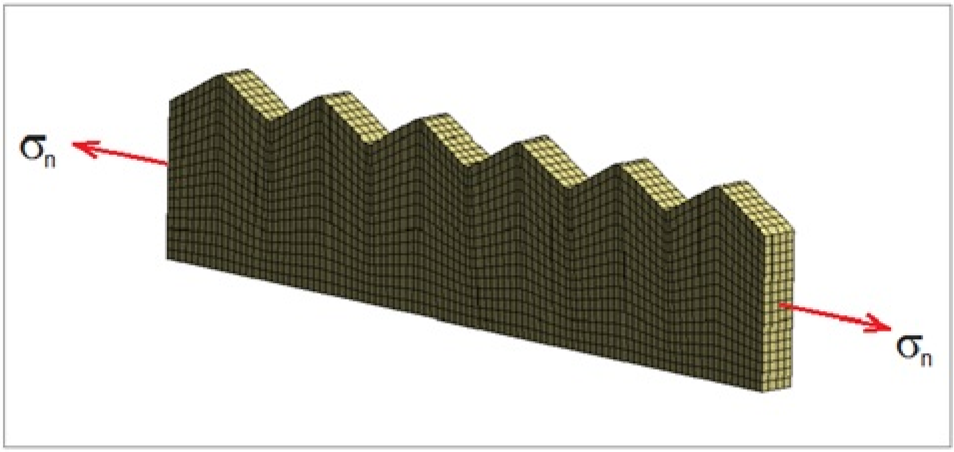

Figure 1: Mesh and scheme of loading used for 3D mapping of stress distribution by FEM.

Methodology of simulation of X-ray diffraction line applied for study of influence of surface roughness on stress measurements is similar to the one used for analysis of surface stress gradients [6]. The methodology is based on composition of total diffraction profile by the sum of individual profiles obtained from any small area dA. This area can be characterized by the depth coordinate t determined as the depth from slope surface of the roughness peak and by local stress σ acting on this area. Fig.2 shows these parameters on the map of stress distribution obtained by FEM.

Calculation of diffracted intensity dI_{dif} generated by area dA can be made on the base of well known equation for attenuation of X-rays into material on the path z:

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

where z is the path for X-ray beam, μ is linear absorption coefficient of X-rays for analyzed material. Path z in the case of X-ray diffraction depends on the depth t and ψ, θ, where ψ is inclination angle between incident beam and normal to the surface of material and θ is diffraction angle. Relationships between these parameters are shown in Fig.3a and can be expressed as:

$$\mathrm{z} = \mathrm{t} * (1/cos(\psi + 90 - \theta) + 1/cos(\psi - 90 + \theta)) \tag{2}$$

In this case intensity dI_{dif} can be write as:

$$\mathrm{dI_{dif}} = kI_0 e^{-\mu z} * dA = k * I_0 e^{-\mu t * (1/cos(\psi+90-\theta)+1/cos(\psi-90+\theta))} dA = Q\,(t, \psi, \theta)\, dA \tag{3}$$

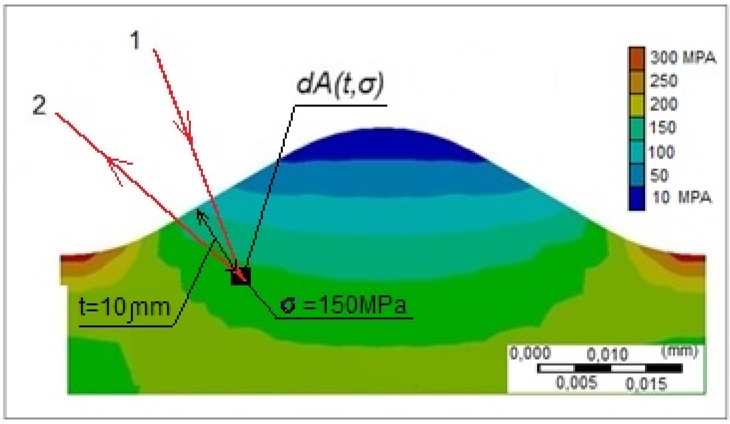

Figure 2: Parameters t and σ of small areas dA on the map of the stress distribution: 1 – incident beam; 2 – diffracted beam.

Here k is proportionality coefficient depending on the crystal structure of material, t is depth of dA from the slope of roughness peak. Fig.3a explains parameters of equations and relationship between equations (1) and (2).

Total intensity of diffracted beam is determined as integral over the surface layer limited by penetration of X-rays into material. For numerical calculation the operation of integration can be substituted by summation over mesh network used for FEM.

Thus, final equation for total diffracted intensity can be calculated as:

$$I_{dif} = \int_0^A Q\left(t, \psi, \theta\right) dA = \sum\nolimits_{n=1}^{N} Q(t, \psi, \theta)\Delta A \tag{4}$$

Fig.3b shows the geometry of diffraction experiment and coordinates used for simulation of diffraction profile for analyzed material. Relationship between stress σ and value of diffraction angle θ can be find from Bragg's law. In the case of uniaxial stress state this relationship can be expressed as:

$$\theta_\psi = \theta_0 - \sigma * (\sin^2\psi - \nu\cos^2\psi)/E * ctg\theta_0. \tag{5}$$

Where E, ν are elastic constants of material, ψ is angle between normal to the analyzed surface and angle bisector for incident and diffracted beams, θ_0 is diffraction angle for unstressed material. For fixed angle ψ equation (4) can be written as principal equation permitting to realize simulation of diffraction profile generated by inhomogeneous stress distribution:

$$I_{dif} = \sum_{n=1}^{N} Q(t, \sigma)\Delta A \tag{6}$$

Besides of simulation of X-ray profiles applied for study of broadening of diffraction lines caused by surface roughness in the present paper it was evaluated possibilities of using of X-ray diffraction method of stress measurements on the rough surface. This method known as "$\sin^2\psi$-method" based on determination of diffraction line positions at different inclinations of X-ray beam to the surface of analyzed material. There are two fundamental equations of this method, one of them describes linear dependence between diffraction

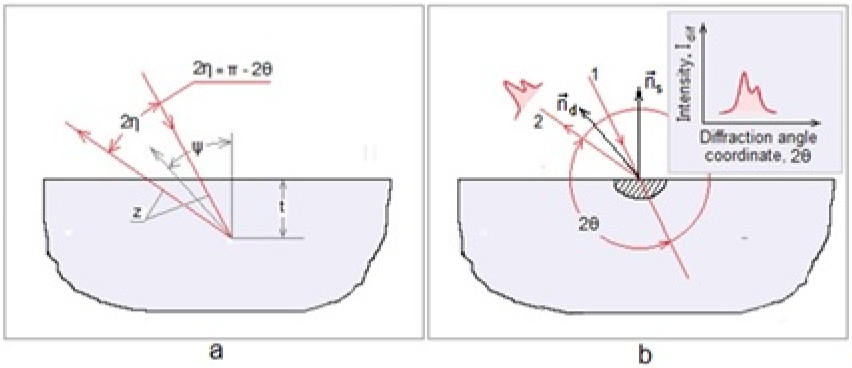

Figure 3: The scheme of passage of incident (1) and diffracted (2) X-ray beems into material (a) and coordinates of profile obtained in diffraction experiment (b).

angle and sine square psi:

$$\theta_\psi = \theta_0 + \sigma_\phi \frac{(1+\nu)}{E} \frac{\sin^2\psi}{ctg\theta} - \frac{\nu}{E}(\sigma_1 + \sigma_2). \tag{7}$$

Other is the formula for stress calculations:

$$\sigma_\phi = \frac{E}{1+\nu} ctg\theta \left(\theta_{\varphi=90} - \theta_{\varphi=0}\right). \tag{8}$$

Scheme in Fig.4 illustrates procedure of stress measurements by "$\sin^2\psi$-method" where diffraction line is determined at series of inclinations of analyzed material to X-ray incident beam.

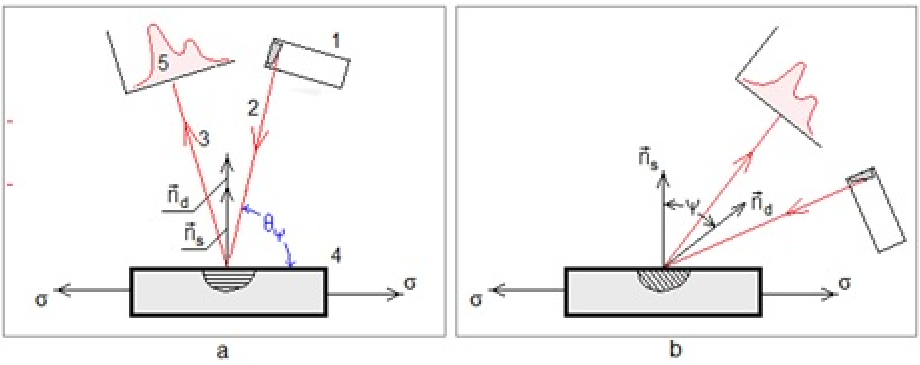

Figure 4: Scheme of X-ray stress measurement by $\sin^2\psi$-method: 1 – X ray tube; 2,3 – incident and diffraction beams; 4 – loaded specimen; 5 – profile of diffraction line; a, b – cases where angle is $\psi = 0$ and $\psi > 0$, respectively.

3 Results and discussion

Carbon steel AISI 1070 was chosen for simulation of loading by tensile force parallel to the surface with introduced roughness. In the present paper there were analyzed specimens with 60^0 and 120^0 v-notches loaded by tensile stress σ equal to 200 MPa. Maps of stress distributions obtained by FEM for are shown in Fig.5,6.

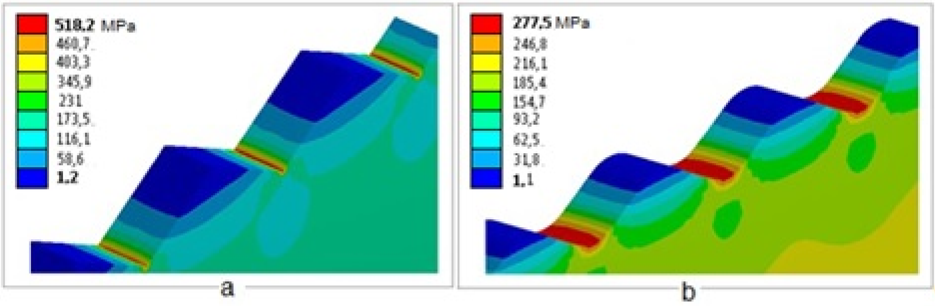

Figure 5: Stress distributions caused by multiple 120^0 v-notch without root radius (a) and with root radius equal to 0,2 mm (b).

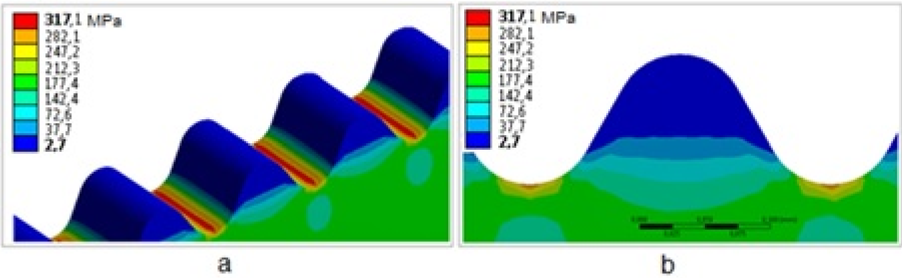

Figure 6: Stress distributions caused by multiple 60^0 v-notch with 0,05 mm root radius: a – general view; b– detailed view.

It can be seen that stress concentrations are localized on the bottom of notches. Highest mean of stress observed at 120^0 v-notch without root radius is equal to 518 MPa (Fig.5a). Less values of stress concentrations are obtained in the case of rounded notches, for example, maximal stress on the bottom of 600 notch with 0,05 mm root radius is equal to 317 MPa. In the case of 120^0 v-notch stress value at the root equals 277 MPa. Opposite, tops of peaks of surface roughness are nearly free from stress action.

One of the difficulties created by surface roughness for stress measurements by X-ray diffraction is limited participation of stress concentration areas in diffraction process. Fig.7 explains situation when increasing of inclination angle ψ decreases diffraction area up to PQ length of blue zone of stress distribution with minimal stress. It is clear that X-ray "$\sin^2\psi$-method" cannot be used for stress measurements here.

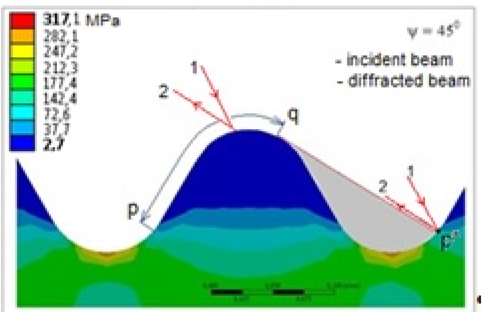

Figure 7: Part of surface roughness peak participating in diffraction process due to shadow effect.

Fig.8 shows positions of X-ray beams for stress measurements when notch angle equals

120 degrees. In this case "$\sin^2\psi$-method" can be used for determination of average stress value. Contribution of every zone is proportional to the area of zone.

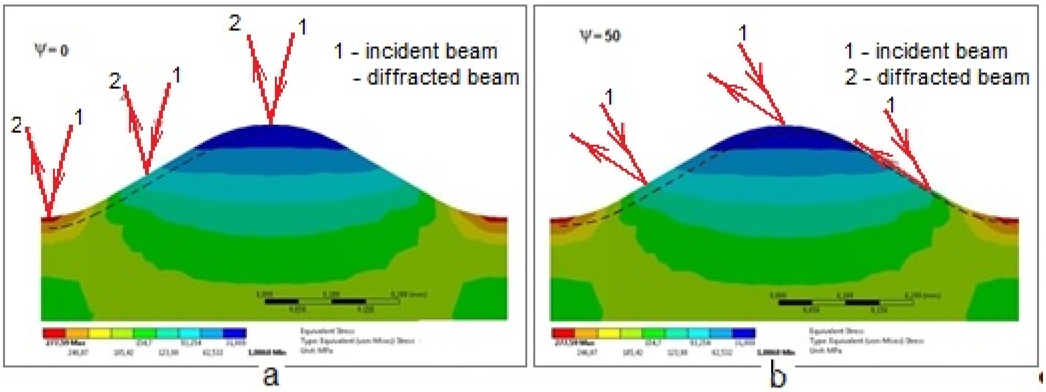

Figure 8: Different positions of X-ray beams towards profile of surface roughness with multiple 120^0 v-notches: a, b – inclination angle of X-ray incidence equals to 0 and 50 degrees, respectively.

Analysis of geometry of stress measurements by X-ray diffraction presented in the Fig.7,8 have been shown that using of "$\sin^2\psi$-method" is limited by notch angle. It can be seen that in the case of small penetration of X-rays into analyzed material and small angle of slope of roughness peak it is impossible to apply "$\sin^2\psi$-method" for stress measurements by X-ray diffraction. In the case of slope angle more than 90 degrees stress state of surface with multiple notches can be measured but experimental results need correlation processing.

Simulation of diffraction profile by surface with inhomogeneous stress distribution gives other opportunity to study surface roughness of materials by X-ray diffraction.

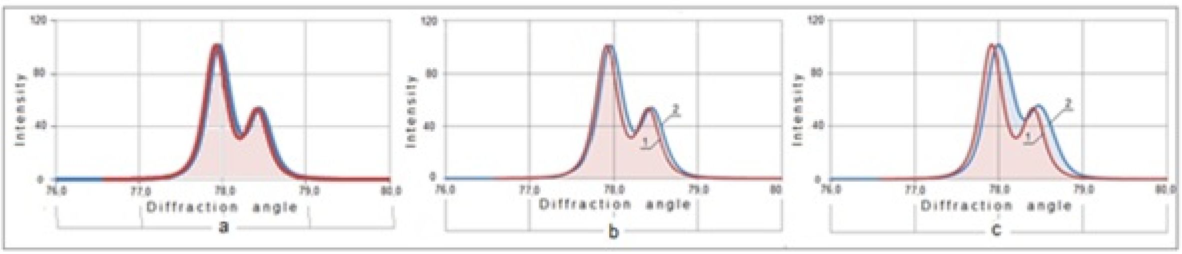

Figure 9: Diffraction profiles formed by smooth surface (1) and surface with multiple v-notches (2): a – 120^0 v-notch with 2 mm root radius; b – 60^0 v-notch with 0,05 mm root radius; c – 120^0 v-notch without root radius.

Using maps of stress distribution obtained by finite element method it can be possible to use developed methodology in simulation of diffraction profiles formed by surface layers with different types of roughness. Fig.8 shows diffraction profiles simulated by surface with multiple v-notches. It can be seen that position and breadth of diffraction profiles depend on stress concentration caused by surface roughness.

4 Conclusion

1. It has been analyzed stress concentrations caused by surface roughness with multiple v-notches. Maps of stress distributions obtained by finite element method were applied for evaluation of surface roughness by simulation of diffraction profiles.

2. It has obtained that broadening of diffraction profiles is proportional to stress concentration caused by surface roughness.

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