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THE EXAMPLE OF TEXTURE INFLUENCE
IN STRESS ANALYSIS

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1. INTRODUCTION

Stress analysis by means of diffraction methods has been developed fast during last years. This is due to the fact that diffraction is the only nondestructive method for internal stress testing of the engineering designs. Moreover, neutron diffraction is the only available method which makes it possible to receive information from the interior of an object. In diffraction experiments the strain is measured directly by analysing peak shift (macro-strains) or peak profiles. To determine the macroscopic stress from mean strain data it is necessary to know the polycrystalline elastic properties. In practice, the texture of a material very often has an influence on the elastic properties and consequently on the resulting stress [1]. In this paper an example of the texture influence on the result of a neutron diffraction stress analysis carried out for the technological sample with cubic crystal symmetry is presented. The diffraction elastic constants (DEC) were calculated by using the geometric mean model [2, 3, 4] taking into account the determined texture [5]. The elastic constants could also be estimated by the self-consistent model [6], which gives the realistic results for isotropic and anisotropic (textured) materials. However, in many cases the bulk means of the elastic constants, determined by self-consistent model or Hill model, are practically identical with those derived by the geometric mean approximation [4]. The advantage of the geometric mean is that the condition for symmetry of “inverse properties” ($S \equiv C^{-1}$) is valid on the macroscopic level for this approximation. Besides, it requires much more simpler calculations than the self-consistent schema, and can be performed for any crystal symmetry and orientation distribution [4]. Therefore it is interesting to compare the results calculated by geometric mean approximations recently developed for stress analysis (“pathgeo”, “bulkpathgeo”) [5] with experimental data.

2. APPROXIMATIONS USED IN STRESS ANALYSIS

2.1 Reuss approximation

In the diffraction stress analysis mean strain is measured for special subset of grains in

a polycrystalline sample. This subset $p = p(\vec{h}_i, \vec{y})$ is determined by the following condition: $\vec{h}_i \parallel \vec{y}$, where $\vec{y}$ is the direction given in the sample coordinate system K_A (Fig. 1) and coinciding with the scattering vector and $\vec{h}_i$ is the normal to the scattering plane given in the crystal coordinate system K_B . So the measured strain in a laboratory system K_L (Fig. 1) depends on the strains of the grains with orientations $g_p = \{\vec{h}_i, \vec{\varphi}\}^{-1} \{\vec{y}, 0\}$, $0 \leq \varphi \leq 2\pi$ [5] which belong to a path p in the three-dimensional orientation space G and weighted by orientation distribution function (ODF) $f(g)$ [5]:

$${}^L\epsilon_{33}(\vec{h}_i, \vec{y}) = \int_0^{2\pi} {}^L\epsilon_{33}(g_p(\varphi)) f(g_p(\varphi)) d\varphi \bigg/ \int_0^{2\pi} f(g_p(\varphi)) d\varphi. \quad (1)$$

Fig. 1. Definition of the laboratory coordinate system K_L , sample coordinate system K_A and the angles φ and ψ .

Using Hooke's law of elasticity we can express the local strain ${}^L\epsilon_{33}(g_p(\tilde{\varphi}))$ by the local stress $\sigma(g_p(\tilde{\varphi}))$. From the other hand, in order to determine the macroscopic stresses in K_A from the measured strain the compliances ${}^LS(p) = {}^LS(\vec{h}_i, \vec{y})$ - diffraction elastic constants (DEC) must be known [7]:

$${}^L\epsilon_{33}(\vec{h}_i, \vec{y}) = {}^LS_{33mn}(\vec{h}_i, \vec{y}) \sigma_{mn}^L = {}^LS_{33mn}(\vec{h}_i, \vec{y}) \{\vec{y}, 0\}_{mk} \{\vec{y}, 0\}_{nl} \sigma_{kl}^A. \quad (2)$$

To determine macroscopic stress it is necessary to involve some assumptions which make the solution simpler. The simplest Reuss assumption rather often used in stress analysis states that stress in each grain is equal to stress applied to the polycrystal. It means that σ does not depend on g_p . The expression for DEC of textured sample in Reuss approximation was obtained in [7]. Matthies rewrote this expression reducing the complicate $f(g)$ -related part to the “moment pole figures” J_q [7]:

$${}^L S_{3311}(\bar{h}_i, \bar{y}) = (U_{11} + U_{22})\mathcal{J}_0(\bar{h}_i, \bar{y})/2 + (U_{11} - U_{22})\mathcal{J}_3(\bar{h}_i, \bar{y})/2 + U_{12}\tilde{\mathcal{J}}_4(\bar{h}_i, \bar{y}), \quad (3a)$$

$${}^L S_{3322}(\bar{h}_i, \bar{y}) = (U_{11} + U_{22})\mathcal{J}_0(\bar{h}_i, \bar{y})/2 - (U_{11} - U_{22})\mathcal{J}_3(\bar{h}_i, \bar{y})/2 - U_{12}\tilde{\mathcal{J}}_4(\bar{h}_i, \bar{y}), \quad (3b)$$

$${}^L S_{3333}(\bar{h}_i, \bar{y}) = U_{33}\mathcal{J}_0(\bar{h}_i, \bar{y}), \quad (3c)$$

$${}^L S_{3323}(\bar{h}_i, \bar{y}) = U_{23}\mathcal{J}_1(\bar{h}_i, \bar{y}) - U_{13}\tilde{\mathcal{J}}_2(\bar{h}_i, \bar{y}), \quad (3d)$$

$${}^L S_{3312}(\bar{h}_i, \bar{y}) = U_{12}\tilde{\mathcal{J}}_3(\bar{h}_i, \bar{y}) - (U_{11} - U_{22})\mathcal{J}_4(\bar{h}_i, \bar{y})/2, \quad (3e)$$

$${}^L S_{3313}(\bar{h}_i, \bar{y}) = U_{13}\tilde{\mathcal{J}}_1(\bar{h}_i, \bar{y}) + U_{23}\mathcal{J}_2(\bar{h}_i, \bar{y}); \quad (3f)$$

$$J_q = \int_0^{2\pi} M_q(\varphi) f(\{\bar{h}_i, \varphi\}^{-1} \{\bar{y}, 0\}) d\varphi / (2\pi\tilde{P}), \quad (4)$$

where $M_0 = 1, M_1 = \cos\varphi, M_2 = \sin\varphi, M_3 = \cos 2\varphi, M_4 = \sin 2\varphi$; $\tilde{P}$ is reduced pole figure [8], $U_{kl}(\bar{h}_i)$ is the part depending on single crystal compliances ${}^0 S_{ruvw}$ given in K_B [7]:

$$U_{kl}(\bar{h}_i) = {}^0 S_{33kl}(\bar{h}_i) = \{\bar{h}_i, 0\}_{3r} \{\bar{h}_i, 0\}_{3u} \{\bar{h}_i, 0\}_{kv} \{\bar{h}_i, 0\}_{lw} {}^0 S_{ruvw}, \quad (5)$$

$$J_q = [J_q(\bar{h}_i, \bar{y}) + J_q(-\bar{h}_i, \bar{y})]/2, \tilde{J}_q = [J_q(\bar{h}_i, \bar{y}) - J_q(-\bar{h}_i, \bar{y})]/2. \quad (6)$$

The introduction of the “moment pole figures” clarifies some properties of ${}^L S_{33mn}(\bar{h}_i, \bar{y})$. For example, the term ${}^L S_{3333}(\bar{h}_i, \bar{y})$ (Eq. 3(c)) does not depend on texture because of $\mathcal{J}_0 = [J_0(\bar{h}_i, \bar{y}) + J_0(-\bar{h}_i, \bar{y})]/2 \equiv 1$ [7]. Beside it is shown in [7] that $J_q = 0$ and as a consequence $\mathcal{J}_q = 0, \tilde{\mathcal{J}}_q = 0$ for $q \neq 0, \bar{h}_i = (001)$ and $\bar{h}_i = (111)$ in case of cubic

materials. That's why all terms ${}^L S_{33mn}(\bar{h}_i, \bar{y})$ do not depend on texture for these cases. So there are situations when it is not possible to take texture into account using Reuss approximation for calculation DEC. The problem connected to disappearance of the texture related terms in expressions for DEC in mentioned cases can arise because Reuss approximation uses too simple arithmetic mean scheme in averaging of DEC ${}^L S$ along orientation path p . The arithmetic mean over all orientations is the simplest approximation to calculate the elastic constants (compliances S or stiffnesses C) of polycrystal with texture described by ODF $f(g)$ and single crystal properties ${}^0 S$ [1]:

$$\bar{S}_{i_1 i_2 j_1 j_2}^a = \int_G g_{i_1 i_1} g_{i_2 i_2} g_{j_1 j_1} g_{j_2 j_2} f(g) dg {}^0 S_{i_1 i_2 j_1 j_2}, \quad (7)$$

where g_{ij} are direction cosines of crystal axis j respect to the axis i of sample coordinate system. However, the arithmetic mean does not provide the equality of “inverse properties” ($S \equiv C^{-1}$) on the macroscopic level [2]:

$$\bar{S} = (\bar{C})^{-1}. \quad (8)$$

2.2 Geometric mean

The condition (8) is exactly realized on the macroscopic level in the frame of geometric mean [2]. The method to calculate elastic properties of textured polycrystals within the frame of geometric mean approach was proposed in [4]:

$$\bar{S}^{GEO} = \exp\{\overline{WW}^a : Ln {}^0 S\}, \text{ where} \quad (9)$$

$$\overline{WW}^a(i_1 i_2, j_1 j_2; i_1' i_2', j_1' j_2') = \int_G W(i_1 i_2, i_1' i_2'; g) W(j_1 j_2, j_1' j_2'; g) f(g) dg. \quad (10)$$

In Eq. 10 $W(i_1 i_2, i_1' i_2'; g) = g_{i_1 i_1} g_{i_2 i_2}$ (Eq. 7), $f(g)$ is ODF and ${}^0 S$ are single crystal properties. In stress analysis the geometric mean (“pathgeo”) was introduced in [5]:

$${}^L S^{p, GEO} = \exp\{\overline{WW}^p : Ln {}^0 S\}, \text{ where} \quad (11)$$

$$\begin{aligned} \overline{WW}^p(i_1 i_2, j_1 j_2; i_1' i_2', j_1' j_2') = \\ = \int_0^{2\pi} W(i_1 i_2, i_1' i_2'; g_p(\varphi)) W(j_1 j_2, j_1' j_2'; g_p(\varphi)) f(g_p(\varphi)) d\varphi \bigg/ \int_0^{2\pi} f(g_p(\varphi)) d\varphi. \end{aligned} \quad (12)$$

In Eq. 11 0S are single crystal compliances. The “pathgeo” have the limitation because it takes into account only the influence of grains belonging to a given path. The bulk path geometric mean “bulkpathgeo” $^L\bar{S}^p$ also introduced in [5] not only obeys $\bar{S} = (\bar{C})^{-1}$ but also takes into account the influence of all grains, represented by bulkgeo-values $\bar{S}^{GEO}$ (Eq. 9):

$$^L\bar{S}^p = ^L S^{GEO} \left[^L\bar{S}^p \right]^{-1} ^L S^{p,GEO}, \quad (13)$$

where $^L S^{GEO}$ is the $\bar{S}^{GEO}$ (Eq. 9) described in K_L . Eq. 13 can be resolved iteratively with Reuss approximation as a starting point.

3. EXPERIMENTAL

The aim of the realized experiment is the examination of different approximations introduced in stress analysis. As a model sample it was chosen the extruded pure Cu rod. The loading and the texture experiments were carried out using neutron diffraction at the spectrometer TEX-2, GKSS, Germany [9]. The orientation distribution function was reconstructed from the three measured complete pole figures (111), (200), (220) by means of three different methods: iterative series expansion method [10], WIMV (Williams-Imhof-Matthies-Vinel) method [11] and texture component method [12, 13]. These results had been already reported [14]. WIMV method gave the best ODF in this case [14]. The sample has rather strong axial texture (Fig.2).

The sample for the loading experiment had cylindrical shape (diameter < 7 mm, height < 36 mm). The loading experiment was practiced according to uniaxial tensile scheme and the condition $Z_L \parallel Z_A$ was valid. It means that tensile was carried out along with extrusion direction. Moreover, the neutron scattering vector coincided with the applied stress. A volume size analysed by neutrons was about 400 mm³. It was considered the

Fig. 2. Experimental pole figures for extruded Cu rod measured by neutron diffraction at TEX-2. Pole figure (111), norm = 6309, contours are 1.5, 3.0, 4.5, 6.0, 7.5 mrd; pole figure (200), norm = 3311, contours are 1.2, 1.8, 2.4, 3.0, 3.6 mrd, pole figure (220), norm = 3052, contours are 0.5, 1.0, 1.5, 2.0, 2.5 mrd

deformation of crystal planes (111) and (200). The sample was subjected to a previous plastic strain (extrusion) so in second loading (tensile test after extrusion) it revealed the strain-stress curve with elastic region up to approximately 380 MPa. That is why there was the possibility to load this sample in the tensile experiment up to 300 MPa in elastic region. The experiment described in this paper is devoted to testing of “pathgeo” and “bulkpathgeo” approximations. Therefore it was chosen for this experiment the strongly elastically anisotropic (pure copper) and strongly textured material with large elastic region in stress-strain curve.

4. RESULTS AND DISCUSSION

The experimental stress-strain curves for the planes (111) and (200) are shown on Fig. 3. On this figure the curves calculated according to Reuss approximation for the planes (111) and (200), according to “pathgeo” approximation and “bulkpathgeo” approximation for the planes (111), (200) and (311) are presented as well. The Reuss

Fig.3. The stress-strain curves for extruded Cu rod in the elastic region measured by neutron diffraction at TEX-2 and calculated in Reuss approximation for the planes (111), (200), and in approximation of textured material ("pathgeo" and "bulkpathgeo" models) for the planes (111), (200), (311).

approximation does not take texture into account for the described experiment. Strain measured along the applied stress in uniaxial tension can be expressed through the only term ${}^L S_{3333}(\vec{h}_i, \vec{y})$ for $Z_L \parallel Z_A$. However, as it has already emphasized, ${}^L S_{3333}(\vec{h}_i, \vec{y})$ in Reuss approximation does not depend on texture. The experimental curves shown on Fig. 3 are in bad conformity with the ones calculated without taking texture into account (Reuss approximation) and according to "pathgeo" approximation. The calculations according to Reuss, "pathgeo" and "bulkpathgeo" approximations were carried out for three different orientations of laboratory K_L and sample coordinate system K_A : 1) $Z_L \parallel Z_A$ ($\varphi = 0^\circ$, $\psi = 0^\circ$), 2) $Z_L \parallel Y_A$ ($\varphi = 90^\circ$, $\psi = 90^\circ$), 3) $Z_L \parallel \vec{R}$, where $\vec{R}$ is the direction in the plane perpendicular to the extrusion direction, $\angle(\vec{R}Y_A) = 45^\circ$ ($\varphi = 45^\circ$, $\psi = 90^\circ$). These calculations aimed at quantitative evaluating of the texture influence on elastic constant in the frame of different approximations. The density of

the plane normals (pole density) coinciding with Z_L in the cases enumerated above is different because of texture (Table 1 and Fig.2). In Table 1 the numerical results for the ${}^L S_{3333}(\vec{h}_i, \vec{y})$ calculated according to three different approximations for the planes (111), (200), (311) and three orientations K_L with regard to K_A are presented.

Table 1. Diffraction elastic constant ${}^L S_{3333}$ obtained from the experiment and calculated according to different models.

(hkl)	K_L relative to K_A	Pole density	${}^L S_{3333}, 10^2 \text{GPa}^{-1}$			
			Reuss	“pathgeo”	“bulkpathgeo”	experiment
(111)	$\varphi = 0^\circ, \psi = 0^\circ$	8.85	0.523	0.523	0.622	0.63 ± 0.02
	$\varphi = 45^\circ$ $\psi = 90^\circ$	0.414	0.523	0.523	0.636	
	$\varphi = 90^\circ$ $\psi = 90^\circ$	0.295	0.523	0.523	0.631	
(200)	$\varphi = 0^\circ, \psi = 0^\circ$	3.69	1.499	1.499	1.050	1.06 ± 0.01
	$\varphi = 45^\circ$ $\psi = 90^\circ$	1.172	1.499	1.499	1.074	
	$\varphi = 90^\circ$ $\psi = 90^\circ$	0.655	1.499	1.499	1.065	
(311)	$\varphi = 0^\circ, \psi = 0^\circ$	1.083	1.039	0.899	0.817	
	$\varphi = 45^\circ$ $\psi = 90^\circ$	0.896	1.039	0.902	0.837	
	$\varphi = 90^\circ$ $\psi = 90^\circ$	0.894	1.039	0.903	0.830	

The table shows that there are limitation not only for Reuss approximation but also for “pathgeo” model which is not able to take texture into account properly for cubic crystal symmetry and $\vec{h}_i = (200)$, $\vec{h}_i = (111)$ in the case of uniaxial test and coinciding of the scattering vector with applied stress. Besides, in the Table 1 the values for ${}^L S_{3333}(\vec{h}_i, \vec{y})$ obtained from the experiment are presented. As can be seen from this Table, the “bulkpathgeo” approximation considering the influence of all grains gives results the most close to the experimental ones. However, the “bulkpathgeo” model does not take into account the role of grain boundaries, which have an influence on the

properties of the real material. Besides, the model works properly only for the approximately spherical grains. So it can be the reason for some difference between experimental values and results calculated according to “bulkpathgeo” model.

5. SUMMARY

It is shown that Reuss approximation for calculation of diffraction elastic constants can not properly takes texture into account for the particular arrangement of deformation diffraction experiment carried out for cubic material: uniaxial tensile (compression) and coinciding of the scattering vector with applied stress. Besides, it is shown that the “bulkpathgeo” model the more accurate takes texture into account than the “pathgeo” approximation and, as a consequence, describes the elastic behaviour of real material better than the “pathgeo” approximation. This fact is also confirmed by experimental stress-strain curves. These curves measured by neutron diffraction in elastic region for the textured cubic material are in good agreement with the ones calculated with taking texture into account by bulk path geometric mean “bulkpathgeo” model. This is the most real-founded model from those considered in this work because it not only obeys reciprocity condition for matrices of compliance and stiffness in macroscopic level but also takes into account the influence of all grains in material.

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Показано влияние текстуры на кривые деформирования, экспериментально измеренные в упругой области методом дифракции нейтронов для медного стержня, подвергнутого экструзии. Информация о текстуре получена из полюсных фигур, измеренных также методом дифракции нейтронов. Кривые деформирования вычислены с учетом и без учета текстуры материала. Расчеты упругих свойств материала с учетом текстуры проведены в рамках схемы геометрического усреднения. Подтверждены преимущества этой схемы, недавно предложенной для расчетов «дифракционных» упругих постоянных.

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Influence of texture on the stress-strain curves experimentally measured in the elastic region by neutron diffraction of an extruded Cu rod is shown. Texture information is obtained from the pole figures measured by neutron diffraction as well. Stress-strain curves are computed with elastic polycrystalline properties calculated with and without taking texture into account. Calculations of elastic polycrystalline properties with texture are carried out according to geometric mean model. The advantage of geometric mean averaging recently developed for diffraction elastic constant calculation is experimentally confirmed.

The investigation has been performed at the Frank Laboratory of Neutron Physics, JINR and at the GKSS — Research Center (Germany).

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