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# FINITE ELEMENT ANALYSIS OF TEXTURED MATERIALS

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The rate-independent formulation of crystal plasticity based on yield surfaces with rounded-off corners is applied to the elastic-plastic FEM analysis of polycrystals. For an assumed finite element mesh of a macroscopic member, a number of crystalline grains are considered in a neighbourhood of each of the integration points. The approach enables analysis of an elastic-plastic behaviour of the material – on the macroscopic level, and a collateral texture development, and slip systems hardening – on the microscopic one. However, a large number of the considered grains require time-consuming computations. To speed up the calculations, the model of a textured continuum is introduced instead of that for the aggregate of grains. In this model, all local fields are *continuous* functions of six variables describing the position of a macroscopic point and the orientation of a microscopic crystalline frame. The FEM procedure is the same as that for the discrete model, but the number of numerical operations decreases about 50 times. The model is fully constrained, i.e. it works under the Taylor assumption, when the local deformation fields are the same as the global one.

*Key words:* finite elements, polycrystals, textural continuum

## 1. Introduction

Investigation of the plastic anisotropy induced during real metal forming processes requires an analysis of the crystallographic texture development in plastically deformed materials (Bacroix et al. (1992)). The basis of the analysis is the single crystal plasticity applied to description of a polycrystal behaviour. In the classical rate-independent crystal plasticity (Hill and Rice (1972)), the problem of ambiguity in the choice of active slip systems appears. For that reason, in practical calculations, the numerical analysis of polycrystals is based on the rate-dependent crystal plasticity (cf Asaro and Needleman (1985)). Such an approach to the modeling of crystallographic texture

development was proposed by Mathur and Dawson (1989). Recently, a rate-independent description of elastic-plastic crystal behaviour, convenient for numerical analysis, was proposed by Gambin (1992a). Instead of the Schmid law, a class of smooth nonlinear yield conditions has been investigated. The corresponding yield surfaces have rounded-off corners. The curvature of corners is determined by a dimensionless material parameter $m > 1.0$. In engineering practice the most popular are f.c.c. (face cubic crystalline) and b.c.c. (body center crystalline) materials. For f.c.c. materials, $m$ is suggested to be equal $(0.5\gamma/Gb) \cdot 10^{-3}$, where $\gamma$ is the stacking fault energy, $G$ is the Kirchhoff modulus and $b$ is the Burger vector modulus (cf Gambin and Barlat (1993)). The proposed model is described by the complete system of equations, and its constitutive relations have the same form as those in the continuum plasticity (McMeeking and Rice (1975)), which makes it possible to adapt the standard finite element procedures to the three-dimensional elastic-plastic analysis of polycrystals (Teodosiu and Gambin (1993)). The analysis includes the collateral observation of global plastic yield, texture evolution and hardening the on the slip systems. The appropriate algorithm is discussed in the present paper. The discussed approach requires repetition of the same calculations for a large number of grains (the standard experimental data contain over 2000 grain orientations). To save the time of computations, Gambin (1992b) and (1993a,b) proposed the use of continuum approach to a description of polycrystal behaviour. In this approach, instead of the analysis of local fields for a large number of grains, the investigation of these fields in the continuous space of the Euler angles $(\varphi_1, \Phi, \varphi_2)$ is carried out. The space of the Euler angles is denoted by $\mathcal{F}^3$, and the corresponding global fields are calculated as mean values of the local ones. Numerical integration over the space $\mathcal{F}^3$ is executed with the help of Gaussian quadrature formulas. The number of integration points in $\mathcal{F}^3$ is much smaller than the relative number of grain orientations in the discrete approach. The procedure of elastic-plastic analysis of polycrystals for the continuum approach, and under the Taylor assumption, is the same as that for the discrete approach, but the number of numerical operations decreases about 50 times.

## 2. Formulation of single crystal plasticity

Recall main results of the formulation of single crystal plasticity proposed by Gambin (1992a). Consider a crystal with $M$ slip systems in the frame of reference. Each of the slip systems is described by the slip direction $\hat{s}_i^{(\alpha)}$

and normal to the slip plane $\hat{m}_i^{(\alpha)}$, for $\alpha = 1,2,...,M$. Elastic properties of the crystal are defined by the matrix of elastic moduli $\hat{\mathcal{L}}_{ijkl}$, while the plastic ones by the matrix of hardening moduli $h_{\alpha\beta}$ $(\alpha,\beta = 1,2,...,M)$, the critical resolved shear stresses $\tau_c^{(\alpha)}$ (for each slip systems) and the discussed previously material parameter $m$. As it was mentioned, one can assume $m = (0.5\gamma/Gb)\cdot 10^{-3}$ for f.c.c. materials. For materials with high stacking fault energy (e.g. aluminium), when $m \geq 30$, crystal behaviour is very close to that described by the classical rate-independent formulation.

In the current configuration, the slip systems of rotated crystal are described by the unit vectors $s_i^{(\alpha)}$ and $m_i^{(\alpha)}$ corresponding to $\hat{s}_i^{(\alpha)}$ and $\hat{m}_i^{(\alpha)}$, respectively. The tensor $\hat{\mathcal{L}}_{ijkl}$ rotated to the current configuration is denoted by $\mathcal{L}_{ijkl}$. Introduce the following auxiliary quantities

$$\begin{aligned} \hat{P}_{ij}^{(\alpha)} &= \frac{1}{2}(\hat{s}_i^{(\alpha)}\hat{m}_j^{(\alpha)} + \hat{m}_i^{(\alpha)}\hat{s}_j^{(\alpha)}) \\ \hat{W}_{ij}^{(\alpha)} &= \frac{1}{2}(\hat{s}_i^{(\alpha)}\hat{m}_j^{(\alpha)} - \hat{m}_i^{(\alpha)}\hat{s}_j^{(\alpha)}) \end{aligned} \tag{2.1}$$

in the reference frame, denoted by $P_{ij}^{(\alpha)}$ and $W_{ij}^{(\alpha)}$ in the current configuration.

Stress state on the slip systems is determined by the resolved shear stress $\tau^{(\alpha)} = \sigma_{ij}P_{ij}^{(\alpha)}$, where $\sigma_{ij}$ is the Cauchy stress tensor. For the constitutive analysis, it is convenient to use the Kirchhoff stress tensor $\tau_{ij} = (\rho/\rho_0)\sigma_{ij}$, where $\rho$ and $\rho_0$ are the mass densities in the current and reference configurations, respectively. A stress increment is assumed to be the Zaremba-Jaumann derivative of the Kirchhoff stress

$$\tau_{ij}^{\nabla} = \dot{\tau}_{ij} - \omega_{ik}\tau_{kj} + \tau_{ik}\omega_{kj} \tag{2.2}$$

where

$\dot{\tau}_{ij}$ – material derivative of $\tau_{ij}$

$\omega_{ij}$ – total material spin.

As the conjugate strain rate measure, the strain rate tensor $d_{ij}$ is taken.

Constitutive behaviour of the discussed model of crystals is described by the following complete system of equations:

— Smooth, nonlinear yield criterion

$$\sum_{\alpha=1}^{M}\left|\frac{\tau^{(\alpha)}}{\tau_c^{(\alpha)}}\right|^m = \frac{1}{M}\sum_{\alpha=1}^{M}\sum_{\beta=1}^{M}\left|\frac{\tau_c^{(\beta)}}{\tau_c^{(\alpha)}}\hat{P}_{ij}^{(\beta)}\hat{P}_{ij}^{(\alpha)}\right|^m \tag{2.3}$$

— Flow rule

$$\tau_{ij}^{\nabla} = \left(\mathcal{L}_{ijkl} - \kappa\frac{\mathcal{F}_{ij}\mathcal{F}_{kl}}{\mathcal{F}_{mn}\mathcal{G}_{mn} + h_0}\right)d_{kl} \tag{2.4}$$

— Constitutive relation for the plastic spin

$$\omega_{ij}^{P} = \Big(\frac{\mathcal{F}_{kl}d_{kl}}{\mathcal{F}_{mn}\mathcal{G}_{mn} + h_0}\Big)\mathcal{H}_{ij} \tag{2.5}$$

— Hardening rule

$$\dot{\tau}_c^{(\alpha)} = \frac{\mathcal{F}_{kl}d_{kl}}{\mathcal{F}_{mn}\mathcal{G}_{mn} + h_0} \sum_{\alpha=1}^{M} h_{\alpha\beta} \frac{1}{\tau_c^{(\beta)}} \Big|\frac{\tau^{(\alpha)}}{\tau_c^{(\beta)}}\Big|^{m-1} \tag{2.6}$$

with the initial values $\tau_c^{(\alpha)} = k_c^{(\alpha)}$ and the hardening moduli matrix

$$h_{\alpha\beta} = h[qI_{\alpha\beta} + (1-q)\delta_{\alpha\beta}] \tag{2.7}$$

where

$I_{\alpha\beta}$ – matrix with all elements equal to one

$\delta_{\alpha\beta}$ – Kronecker symbol

$h$ – constant self-hardening rate (the same for all slip systems)

$q$ – latent hardening ratio.

In Eq (2.4), $\kappa = 1$ for the plastic loading, and $\kappa = 0$ for the other cases. Moreover

$$\mathcal{F}_{ij} = \sum_{\alpha=1}^{M} \frac{\lambda_{ij}^{(\alpha)}}{\tau_c^{(\alpha)}} \Big|\frac{\tau^{(\alpha)}}{\tau_c^{(\alpha)}}\Big|^{m-1} \qquad \mathcal{G}_{ij} = \sum_{\alpha=1}^{M} \frac{P_{ij}^{(\alpha)}}{\tau_c^{(\alpha)}} \Big|\frac{\tau^{(\alpha)}}{\tau_c^{(\alpha)}}\Big|^{m-1} \tag{2.8}$$

$$h_0 = \sum_{\alpha=1}^{M}\sum_{\beta=1}^{M} \frac{h_{\alpha\beta}}{\tau_c^{(\alpha)}\tau_c^{(\beta)}} \Big|\frac{\tau^{(\alpha)}}{\tau_c^{(\alpha)}}\Big|^{m} \Big|\frac{\tau^{(\beta)}}{\tau_c^{(\beta)}}\Big|^{m-1} + \tag{2.9}$$

$$+ \sum_{\alpha=1}^{M}\sum_{\beta=1}^{M}\sum_{\delta=1}^{M} \Big(\frac{h_{\beta\delta}}{\tau_c^{(\beta)}\tau_c^{(\delta)}} - \frac{h_{\alpha\delta}}{\tau_c^{(\alpha)}\tau_c^{(\delta)}}\Big)\Big(2\frac{\tau_c^{(\beta)}}{\tau_c^{(\alpha)}} \hat{P}_{ij}^{(\beta)} \hat{P}_{ij}^{(\alpha)}\Big)^{m} \Big|\frac{\tau^{(\delta)}}{\tau_c^{(\delta)}}\Big|^{m-1}$$

$$\mathcal{H}_{ij} = \sum_{\alpha=1}^{M} \frac{W_{ij}^{(\alpha)}}{\tau_c^{(\alpha)}} \Big|\frac{\tau^{(\alpha)}}{\tau_c^{(\alpha)}}\Big|^{m-1} \tag{2.10}$$

with

$$\lambda_{ij}^{(\alpha)} = \mathcal{L}_{ijkl}P_{kj}^{(\alpha)} + W_{ik}^{(\alpha)}\tau_{kj} - \tau_{ik}W_{kj}^{(\alpha)} \tag{2.11}$$

Eqs (2.2) ÷ (2.11) are sufficient to analyze large plastic strains of elastic-plastic single crystals. The incremental procedure being used requires updating of all vector and tensor quantities to the current crystal configuration according to the lattice reorientation. An appropriate rotation matrix $R_{ij}$ may be

calculated on the base of lattice spin $\omega^*_{ij} = \dot{R}_{ik}R_{jk}$. The spin $\omega^*_{ij}$ is a difference between the total spin $\omega_{ij}$ and the plastic one $\omega^p_{ij}$. The current rotation matrix $R_{ij}$ is determined by three Euler angles $(\varphi_1, \Phi, \varphi_2)$. Their initial values $(\varphi_1^0, \Phi^0, \varphi_2^0)$ define the initial rotation matrix $R^0_{ij}$.

## 3. Finite element analysis of crystal aggregate

Teodosiu and Gambin (1993) applied the above formulation of single crystal plasticity to the finite element analysis of elastic-plastic polycrystals. The analyzed macroscopic system is divided into $N_E$ finite elements with $N_I$ integration points within each element. The material in a small vicinity of each integration point is considered as an aggregate of $N_G$ groups of crystalline grains. All the grains belonging to one of the groups are supposed to have the same initial lattice orientation and the initial critical shear stresses. The alternative approach, proposed by Teodosiu et al. (1993), in which dislocation densities on slip systems, instead of the critical shear stresses are chosen as internal variables, is also included into the discussed work. The analysis is based on the Taylor assumption, when the local deformation fields on each $N_G$ grain are the same. Because constitutive description of the material is given on the microscopic level, the calculations are made within three main loops: over the elements, the integration points and the grains. General strategy of computation is the same as in the standard FEM analysis (cf McMeeking and Rice (1975)). To obtain the explicit scheme of computations, the classical power principle (cf Cao and Teodosiu (1992)) formulated in terms of the global fields is used. The principle referred to the current configuration has the following form

$$\int_V \Big[\Big(\langle \tau^{\nabla}_{ij}\rangle - 2\langle \tau_{ik}\rangle d_{kj}\Big)\delta d_{ij} + \langle \tau_{jk}\rangle v_{i,k}\delta v_{i,j}\Big]\,dV = \int_S \dot{p}_i \delta v_i \, dS \tag{3.1}$$

Assume that

$$\langle A\rangle \equiv \frac{\sum\limits_g \varphi^g A^g}{\sum\limits_g \varphi^g} \tag{3.2}$$

is the mean value of a local field $A^g$ prescribed on the $g$th group of grains and $\varphi^g$ is a volume amount of the $g$th group in the representative volume of polycrystalline material. Using this notation, $\langle \tau^{\nabla}_{ij}\rangle$ is the mean value of the Zaremba-Jaumann derivative of the Kirchhoff stress, and $v_i$, $v_{i,j}$, $d_{ij}$, as well

as, $\dot{p}_i$ represent the global fields of velocity, gradient of velocity and load rate, respectively. By $\delta v_i$, $\delta v_{i,j}$ and $\delta d_{ij}$ the corresponding virtual increments are denoted. $\delta_{ij}$ is the Kronnecker symbol. Introducing Eq (2.4) into (3.1), the virtual power principle takes the form

$$\int_V D_{ijkl} v_{k,l} \delta v_{i,j} \, dV = \int_S \dot{p}_i \delta v_i \, dS \tag{3.3}$$

where

$$D_{ijkl} \equiv \langle C^{ep}_{ijkl} \rangle - \frac{1}{2}\langle \tau_{ik} \rangle \delta_{jl} - \frac{1}{2}\langle \tau_{jk} \rangle \delta_{il} - \frac{1}{2}\langle \tau_{il} \rangle \delta_{jk} + \frac{1}{2}\langle \tau_{jl} \rangle \delta_{ik} \tag{3.4}$$

$$\langle C^{ep}_{ijkl} \rangle \equiv \langle \mathcal{L}_{ijkl} - \kappa \frac{\mathcal{F}_{ij}\mathcal{F}_{kl}}{\mathcal{F}_{mn}\mathcal{G}_{mn} + h_0} \rangle \tag{3.5}$$

For the considered macroscopic system with the polycrystalline structure, a finite element mesh and approximation of the global velocity field by shape functions $N_B$ are assumed

$$v_k = \sum_B N_B v_{Bk} \tag{3.6}$$

where $v_{Bk}$ are the values of $v_k$ at the finite element nodes. Analogicaly, for the virtual velocities

$$\delta v_k = \sum_A N_A \delta v_{Ak} \tag{3.7}$$

Introducing Eqs (3.6) and (3.7) into Eq (3.3), one obtains the FEM system of equations

$$\sum_B K_{AiBk} \delta v_{Bk} = \dot{p}_{Ai} \tag{3.8}$$

where

$$K_{AiBk} \equiv \int_V N_{A,j} D_{ijkl} N_{B,l} \, dV \tag{3.9}$$

$$\dot{p}_{Ai} \equiv \int_S N_A \dot{p}_i \, dS \tag{3.10}$$

are local or global stiffness matrix and global or local load rate vector, respectively, depending the way of integration, i.e. over one element or over the whole system. Because the analysis is incremental, an increment of a displacement $\Delta U$ and an increment of applied forces $\Delta p$ will be used instead of $v_i$ and $\dot{p}_i$, respectively.

The algorithm consists of three stages:
— Formation of the matrix $[K]$ (local and global)
— Formation of the vector $\{\Delta p\}$ (local and global)
— Solving of the system $[K]\{\Delta U\} = \{\Delta p\}$.

The two last stages and formation of the global stiffness matrix are the same as in the standard FEM analysis. Complementation of the matrix $D_{ijkl}$, when the matrix $\langle C^{ep}_{ijkl}\rangle$ is given, is well known (cf McMeeking and Rice (1975)). Our attention will be focused on formation of the mean elastic-plastic matrix $\langle C^{ep}_{ijkl}\rangle$. To calculate this matrix, the following procedure is employed (for notation – see the previous section).

- Initialization
  - introduce the input data:
    - common for all grains (in the reference, isoclinic configuration): $\hat{\mathcal{L}}_{ijkl}$, $\hat{s}_i^{(\alpha)}$, $\hat{m}_i^{(\alpha)}$, (for $\alpha = 1, 2, ..., M$); $k_c$, $h$, $q$; $m$
    - for each grain: $\varphi_1^0$, $\Phi^0$, $\varphi_2^0$; $\varphi^g$
  - calculate input functions:
    - common for all grains (in the reference configuration): $\hat{P}_{ij}^{(\alpha)}$, $\hat{W}_{ij}^{(\alpha)}$
    - for each grain: $R_{ij}^0(\varphi_1^0, \Phi^0, \varphi_2^0)$
- Computation ($i$th step of the incremental procedure $(i \geq 1)$)
  - form the vector of state variables composed of: $\tau_{ij}$, $\tau_c^{(\alpha)}$, $R_{ij}$, for all grains in the current configuration
  - calculate the state vector functions:
    - in the reference configuration: $\hat{\tau}_{ij}$, $\hat{\lambda}_{ij}^{(\alpha)}$, $\tau^{(\alpha)}$; $\hat{\mathcal{F}}_{ij}$, $\hat{\mathcal{G}}_{ij}$, $\mathcal{H}_{ij}$; $h_{\alpha\beta}$, $h_0$, $\kappa$; $C^{ep}_{ijkl}$, for each grain
    - in the current configuration: $C^{ep}_{ijkl} = R_{ip}R_{jq}R_{kr}R_{ls}C^{ep}_{pqrs}$
  - calculate the matrix $\langle C^{ep}_{ijkl}\rangle$
  - solve the system $[K]\{\Delta U\} = \{\Delta p\}$, and next calculate $d_{ij}$ and $\omega_{ij}$
  - update the state vector variables: $\tau_{ij}$, $\tau_c^{(\alpha)}$ and $R_{ij}$, for each grain.

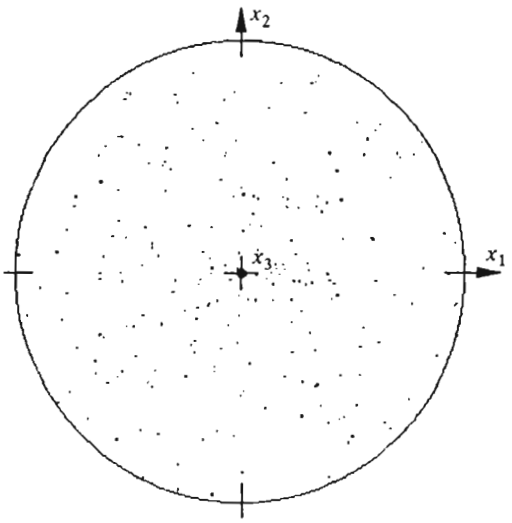


Fig. 1. Initial distribution of 106 grains and the assumed reference frame

## 4. Uniform strain tests for f.c.c and b.c.c. polycrystals

The presented algorythm should be tested both on the macroscopic level and the microscopic one. For testing on the macroscopic level one can use the standard FEM tests. On the microscopic level, lattice grain reorientations during a plastic yield appear. They are responsible for evolution of plastic anisotropy in polycrystalline materials. The lattice reorientation – strain rate relation should be tested too. Below the results of such tests for an aggregate of 106 grains are shown. At the beggining of deformation the aggregate is assumed to be an isotropic one, i.e. the initial lattice orientations are uniformly distributed in the orientation space. The results are presented with the help of (100) and (111) pole figures. The assumed reference frame and the initial distribution of lattice grain orientations are shown in Fig.1. The next figures show lattice reorientations for $m = 30$ and 100% final strain. A virtual strain rate increment is assumed as 2.5%.

The following situations are considered both for f.c.c. and b.c.c. crystal aggregates (non written components of $d_{ij}$ are equal to zero):

– compression with $d_{11} = d_{22} = -0.5$, $d_{33} = -1.0$

– drawing with $d_{11} = d_{22} = -0.5$, $d_{33} = 1.0$

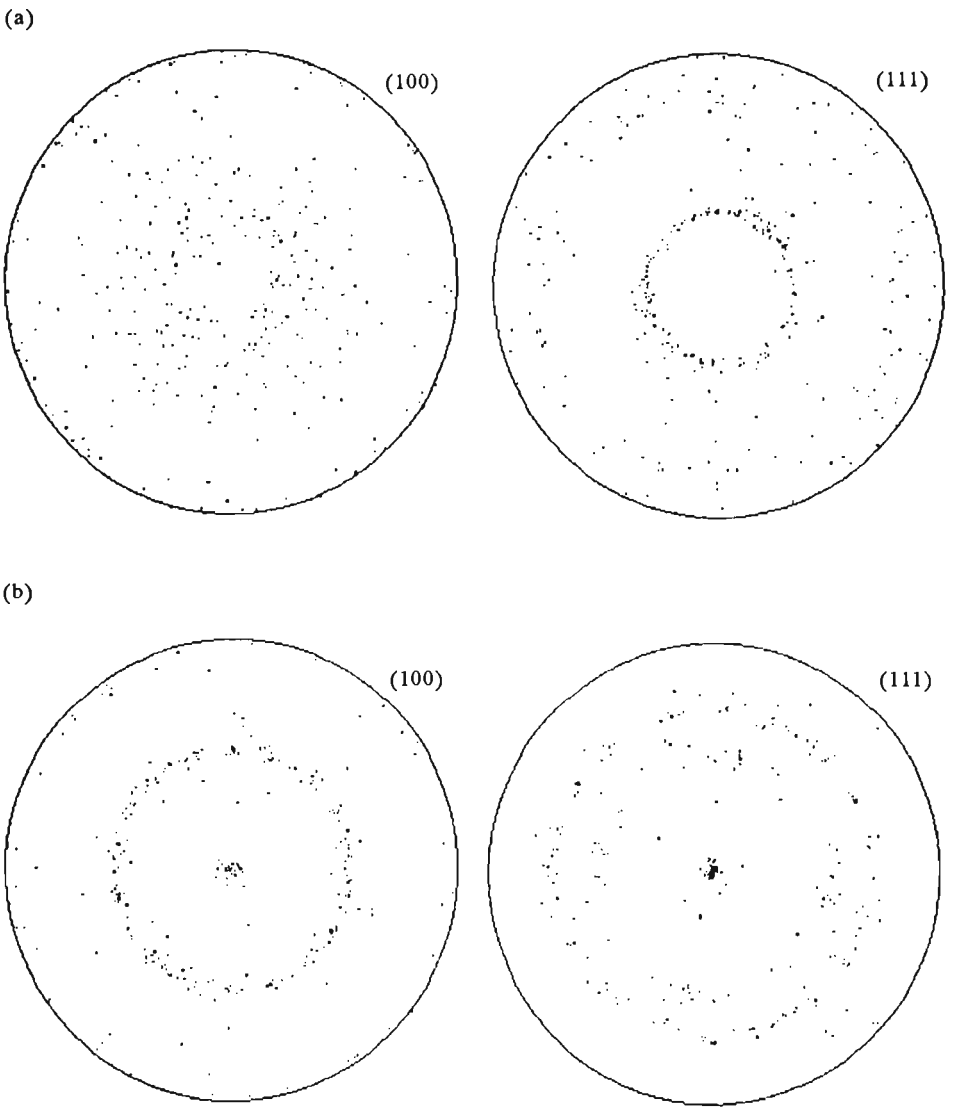


Fig. 2. The (100) and (111) pole figures after 100% strain of 106 f.c.c. grain aggregate: (a) – compressed, (b) – drawn

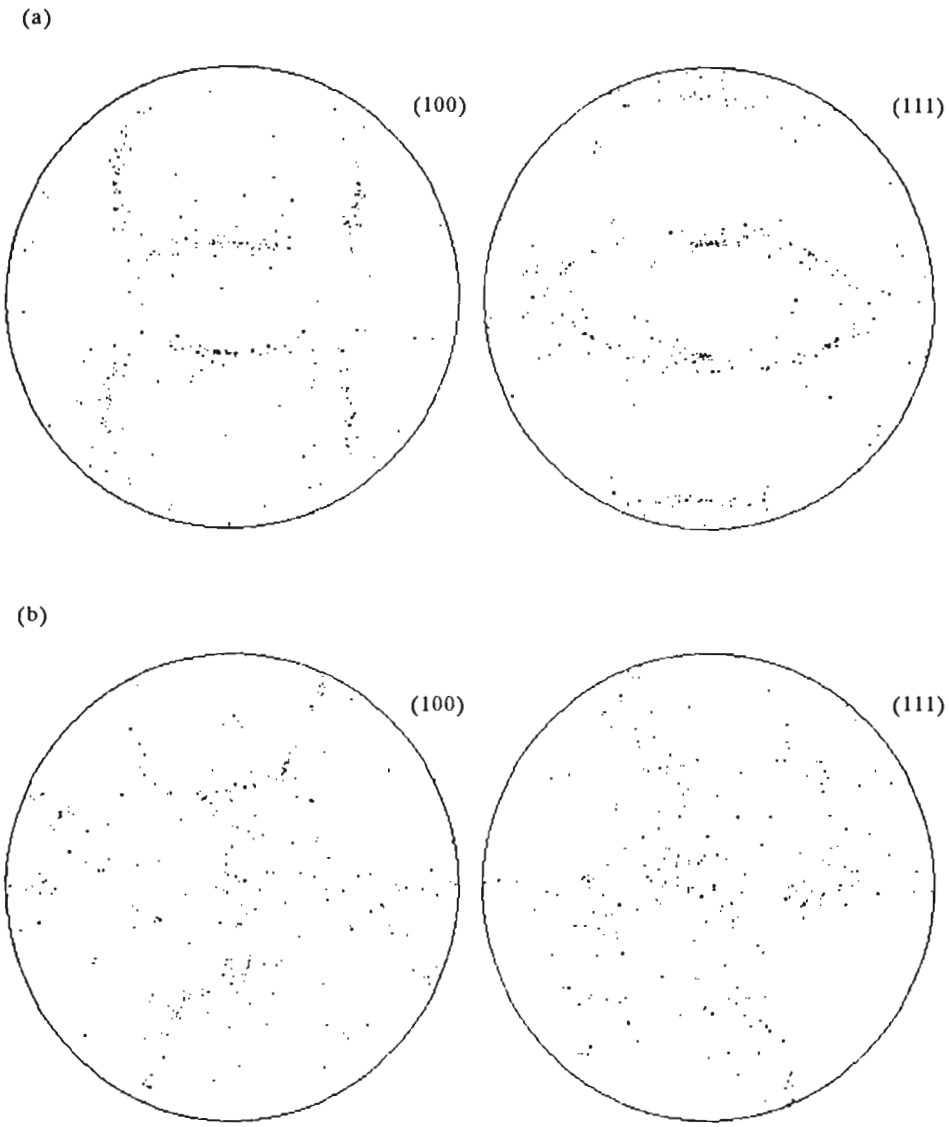


Fig. 3. The (100) and (111) pole figures after 100% strain of 106 f.c.c. grain aggregate: (a) – rolled, (b) – sheared

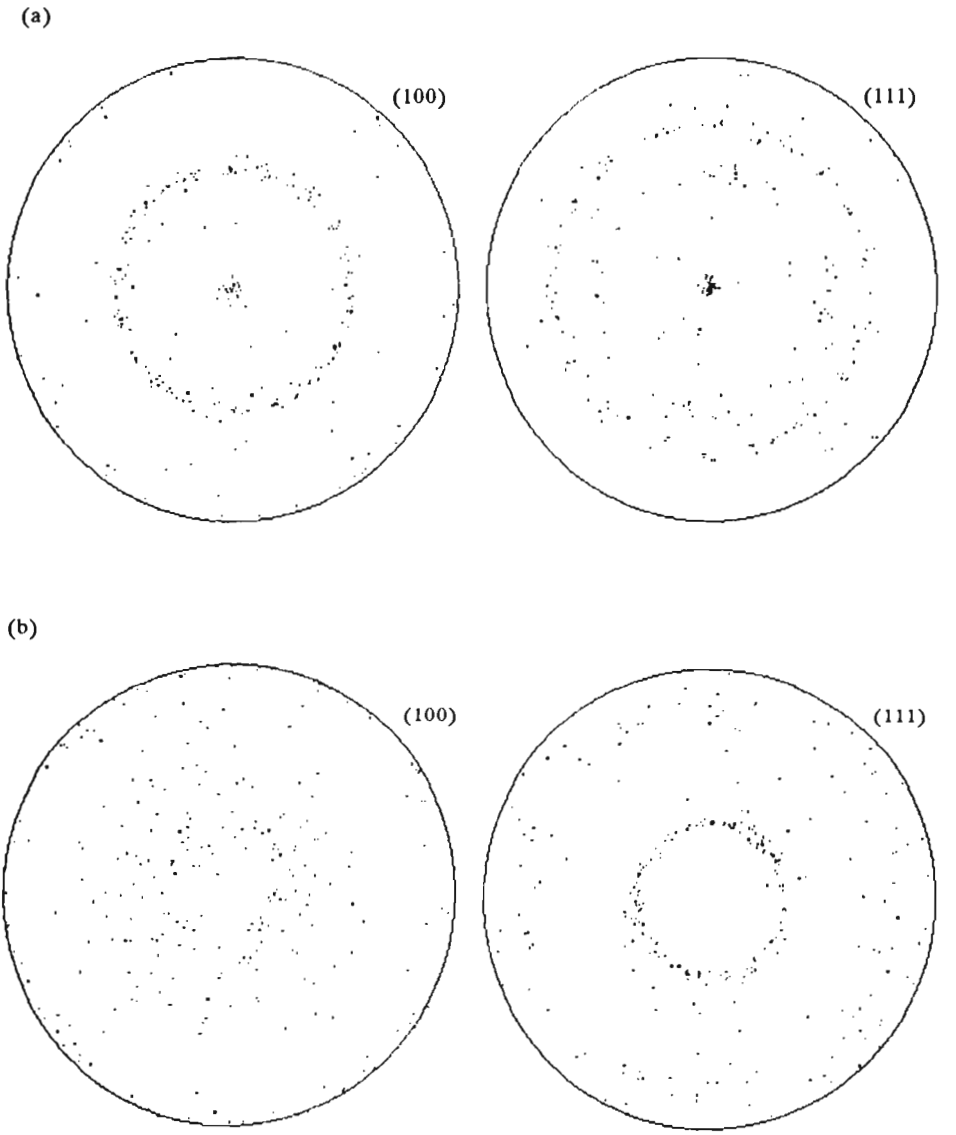


Fig. 4. The (100) and (111) pole figures after 100% strain of 106 b.c.c. grain aggregate: (a) – compressed, (b) – drawn

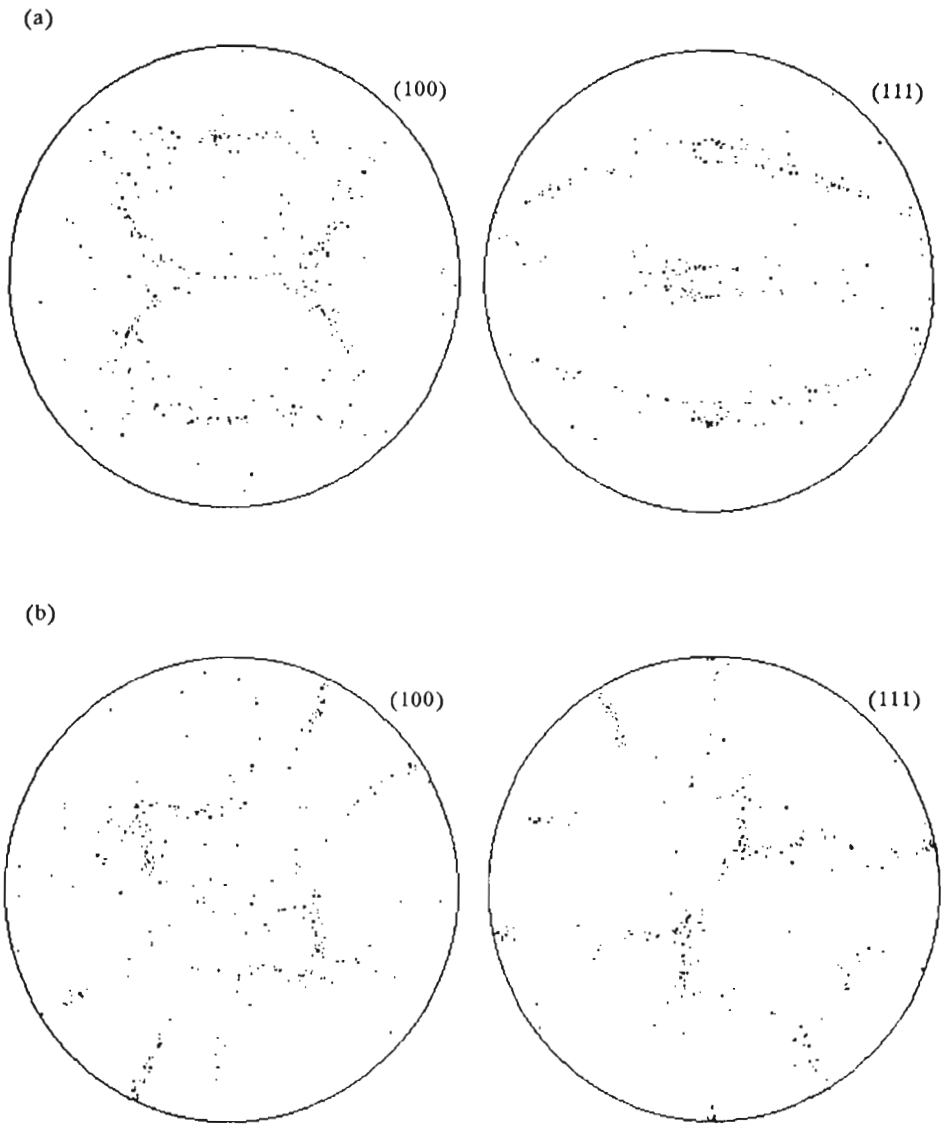


Fig. 5. The (100) and (111) pole figures after 100% strain of 106 b.c.c. grain aggregate: (a) – rolled, (b) – sheared

– rolling with $d_{22} = 1.0$, $d_{33} = -1.0$

– shearing with $d_{12} = 1.0$.

## 5. Textured material as continuous model of polycrystal

Notice, that in our analysis of a microscopic polycrystal behaviour, the grain interactions, their shape, size and spatial distribution around the integration points were neglected. It means that each grain surrounding an integration point was represented by its lattice frame and the associated system of slip systems. Then, on the macroscopic level, one can consider *a continuum of lattice frames* attached to the considered integration point instead of a finite number of grains (cf Gambin (1992b)). Each of these frames may be labelled by its initial orientation $g^0$ belonging to the three-dimensional continuous space of the Euler angles $\mathcal{F}^3$.

Consider such a continuum of lattice frames attached to the macroscopic point $X_k$, which corresponds to a polycrystalline element with the representative volume $V_0^r$, centred at $X_k$. To describe a distribution of initial orientations for the considered continuum, one can take the volume fraction of grains $dV_0^r/V_0^r$ that have the initial orientation $g^0$ within a certain infinitesimal orientation element $dg^0$. This fraction corresponds to the ratio $V_0^g/V_0^r$ in the case of discrete grain distribution. For a given $dV_0^r/V_0^r$, one can introduce a density of lattice frames $F_0(X_k, g^0)$, in the space $\mathcal{F}^3$

$$\frac{dV_0^r}{V_0^r} = F_0(X_k, g^0) dg^0 \tag{5.1}$$

such that

$$\int_{\mathcal{F}^3} F_0(X_k, g^0)\, dg^0 \equiv 1 \tag{5.2}$$

The infinitesimal element $dg^0$ in terms of increments of the Euler angles has the following form

$$dg^0 = \frac{1}{8\pi^2} \sin \Phi^0 d\varphi_1^0 d\Phi^0 d\varphi_2^0 \qquad \begin{cases} 0 \le \varphi_1^0 \le 2\pi \\ 0 \le \Phi^0 \le \pi \\ 0 \le \varphi_2^0 \le 2\pi \end{cases} \tag{5.3}$$

For a fixed point $X_k$, the function $F_0(g_0)$ is called the initial Orientation Distribution Function (ODF) and it plays a fundamental role in the standard texture analysis (cf Cao and Teodosiu (1992)).

Consider a macroscopic material element of the volume $V_0$ and the external surface $S_0$ in the reference configuration. Now, the local fields $\dot{T}^g_{ij}(X_k, g^0)$, $v^g_{i,j}(X_k, g^0)$ and $\dot{p}^g_i(X_k, g^0)$, $v^g_i(X_k, g^0)$ are prescribed on $V_0 \times \mathcal{F}^3$ and $S_0 \times \mathcal{F}^3$, respectively. Because their evolution depends on the texture development only, one can say about the model of *a textured material* introduced in the place of the crystalline aggregate. To extend the virtual power principle (Eq (3.1)) to the case of textured materials, redefine the averaging procedure (Eq (3.2)) applying the rule

$$\langle A \rangle \equiv \int_{\mathcal{F}^3} F_0(X_k, g^0) A(X_k, g^0)\, dg^0 \tag{5.4}$$

which is valid for an arbitrary local field $A(X_k, g^0)$ prescribed on $V_0 \times \mathcal{F}^3$.

## 6. Finite element analysis of textured materials

Following the Taylor model of polycrystals, one can use principle (3.1) with the averaging procedure (Eq (5.4)) to formulate the explicit scheme of the FEM analysis for elastic-plastic textured materials. Recall that principle (3.1) is written in the form referred to the current configuration of a macroscopic element of textured material.

Let $x_k$ be the current position of macroscopic point initially located at $X_k$, and $f_0(x_k, g^0)$ the initial ODF at this point, respectively. If we neglect an influence of elastic strains on the ODF, the representative volume $V_0^r$, at the point $X_k$, does not change during the deformation process. Then, it follows from Eq (5.3)

$$f_0(x_k, g^0) = F_0(X_k, g^0) \tag{6.1}$$

and Eq (5.4) may be written in the equivalent form

$$\langle A \rangle \equiv \int_{\mathcal{F}^3} f_0(x_k, g^0) A(x_k, g^0)\, dg^0 \tag{6.2}$$

In the above, the local field $A(x_k, g^0)$ is prescribed on $V \times \mathcal{F}^3$, where $V$ is the volume of textured material in the current configuration. Eq (5.3) enable us to express the integral over $\mathcal{F}^3$ in terms of the Euler angles. If we restrict the considerations to the crystals with cubic symmetry, the integration may

be limited to the following intervals (cf Hutchinson (1970))

$$\begin{cases} 0 \leq \varphi_1^0 \leq \pi/2 \\ 0 \leq \Phi^0 \leq \pi/2 \\ 0 \leq \varphi_2^0 \leq \pi/2 \end{cases} \tag{6.3}$$

Finally, the averaging procedure for cubic crystals takes the form

$$\langle A \rangle \equiv \frac{4}{\pi^2} \int_0^{\frac{\pi}{2}} \int_0^{\frac{\pi}{2}} \int_0^{\frac{\pi}{2}} f_0(x_k; \varphi_1^0, \Phi^0, \varphi_2^0) A(x_k; \varphi_1^0, \Phi^0, \varphi_2^0) \sin \Phi^0 \, d\varphi_1^0 d\Phi^0 d\varphi_2^0 \tag{6.4}$$

For simplicity, the considerations below will be related to a fixed point $x_k$, i.e. the analyzed fields will be assumed to be functions of their initial orientations only. The integral on the right hand side of Eq (6.4) may be calculated numerically, as the product of Gaussian quadrature formulas for a one-dimensional function $h(x)$ (cf Stroud and Secrest (1966))

$$\int_a^b w(x)h(x) \, dx \simeq \sum_{i=1}^{N} H_i h(x_i) \tag{6.5}$$

where $w(x)$ is an arbitrary weighting function, and the points $x_i$, as well as, the weights $H_i$ are taken such that the rule (6.5) be exact for

$$w(x) = \sum_{k=0}^{2N-1} a_k x^k \tag{6.6}$$

To use the above technique for integration over the space $\mathcal{F}^3$, it is necessary to determine a complete system of functions, in three Euler angles, for which rule (6.5) is fulfilled exactly.

Notice, that an arbitrary analytical field $F$ prescribed on $\mathcal{F}^3$ can be developed in a series of generalized spherical harmonics $T_l^{mn}$ (cf Bunge (1982))

$$F(\varphi_1^0, \Phi^0, \varphi_2^0) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \sum_{n=-l}^{+l} C_l^{mn} T_l^{mn}(\varphi_1^0, \Phi^0, \varphi_2^0) \tag{6.7}$$

The real part of $T_l^{mn}$ is a trigonometric polynomial of the degree $l$. Denote by $F_{(L)}$ the approximation of the field $F$ by the harmonics $T_l^{mn}$, for $l = 0, 1, 2, ..., L$. We are looking for quadrature formulas which are exact for the function $F_{(L)}$. Take into account, that $F_{(L)}$ is a linear combination of

monomials of the $(\cos\varphi)^\alpha \times (\cos\varphi)^\beta$ type, where $\alpha + \beta = L$. Then, after the substitutions

$$\cos\varphi_{1,2}^0 = y_{1,2} \qquad \cos\Phi^0 = y \tag{6.8}$$

one can write the following conversion rules

$$\begin{aligned} \int_0^{\frac{\pi}{2}} \cos^L \varphi_{1,2}^0 \, d\varphi_{1,2}^0 &= \int_0^1 \sqrt{1 - y_{1,2}} y_{1,2}^L \, dy_{1,2} \\ \int_0^{\frac{\pi}{2}} \cos^L \Phi^0 \sin\Phi^0 \, d\Phi^0 &= \int_0^1 y^L \, dy \end{aligned} \tag{6.9}$$

The above relations enable one to express the integral of $F_{(L)}$ as the integral of certain algebraic polynomials $h(y_{1,2})$ and $h(y)$. To integrate them numerically, one can use the following rules (cf Stroud and Secrest (1966))

$$\begin{aligned} \int_0^1 \sqrt{1 - y_{1,2}} h(y_{1,2}) \, dy_{1,2} &= \frac{\pi}{N} \sum_{i=1}^{\frac{N}{2}} \cos\frac{2i-1}{2N}\pi \\ \int_0^1 h(y) \, dy &= \sum_{j=1}^{\frac{N}{2}} H_j h(y_j) \end{aligned} \tag{6.10}$$

where $N$ is even, and $H_j$ and $y_j$ define the $N$-point Gauss-Legendre formula. Concluding, the integral of $F_{(L)}$ can be calculated exactly by the formula

$$\int_{\mathcal{F}^3} F_{(L)} \, dg^0 = \frac{4}{N^2} \sum_{i=1}^{\frac{N}{2}} \sum_{j=1}^{\frac{N}{2}} \sum_{k=1}^{\frac{N}{2}} H_j F_{(L)}\left(\pi\frac{2i-1}{2N}, \arccos y_j, \pi\frac{2k-1}{2N}\right) \tag{6.11}$$

Return to averaging procedure $(6.10)_2$. Consider next the most complex case of calculations: a material is composed of crystals with triclinic symmetry and it has a very strong initial texture. According to Bunge (1982), for crystals with an arbitrary symmetry, the Orientation Distribution Function can be approximated with a sufficient accuracy by a trigonometric polynomial of the degree $l = 22$. It seems reasonable to assume the same degree of approximation for the local field $A(x_k, g^0)$. For exact integration of the product of two approximating polynomials, it is enough to take $N = 22$ in the above rules. This number may be reduced considerably, if the material

is composed of cubic crystals. Then, one can take $N = 6$ (cf Arminjon and Imbault (1993)).

The numerical integration procedure (6.11) enables one to interpret our treatment in terms of the discrete approach (see Eq (3.2)). Around each integration point, one can consider a finite number of grains with the initial orientations

$$g^0 = (\varphi^0_{1(i)}, \Phi^0_{(j)}, \varphi^0_{2(k)}) = \left(\pi\frac{2i-1}{2N}, \arccos y_j, \pi\frac{2k-1}{2N}\right) \tag{6.12}$$

for $i,j,k = 1,2,...,N/2$, where $N$ is even. Introducing the index: $g = i + (j1)N/2 + (k1)(N/2)^2$, the grains may be numbered by: $g = 1,2,...,N_G$, where $N_G = (N/2)^3$. Denote by

$$\varphi^g \equiv H_j f_0(\varphi^0_{1(i)}, \Phi^0_{(j)}, \varphi^0_{2(k)}) \tag{6.13}$$

the weight of $g$th grain. From Eqs (5.2), (6.1) and (6.11), it follows that

$$\sum_g \varphi^g = \frac{N^2}{4} \tag{6.14}$$

Therefore, instead of the local fields $A(g^0)$ on the continuous space $\mathcal{F}^3$, one can take the local fields $A^g$ on the finite set of grains with the initial orientations given by Eq (6.12). Then, averaging procedure (6.4) takes the form (see Eq (3.2))

$$\langle A\rangle = \frac{\sum_g \varphi^g A^g}{\sum_g \varphi^g} \tag{6.15}$$

As we see, the algorithm for explicit scheme of the elastic-plastic FEM analysis for textured materials, under the Taylor assumption, is the same as in the case of crystalline aggregate described previously. However, the number of considered grains has been reduced diminished considerably.

## 7. Concluding remarks

The standard finite element procedures for classical elastic-plastic analysis at large strain can be easily extended to the collateral texture development investigation. The corresponding formulation is based on the refined elastic-plastic analysis of single crystals (cf Gambin (1992a)). A complete system of

equations and the classical form of constitutive relations enable one to adapt the available numerical codes of FEM analysis to the case of crystalline aggregate (cf McMeeking and Rice (1975)). The computations can be improved, if the model of textured continuum instead of the crystalline aggregate is used. In this model, it is assumed that all local fields attached to a macroscopic point, are continuous functions of the position of the considered point and orientation of the local lattice frame. Under the Taylor assumption the model of textured continuum enables us to reduce the number of numerical operations about 50 times. Moreover, generalization of the virtual power principle proposed in paper gives a possibility of analyzing the local deformation fields putting a side the Taylor assumption. Such an analysis is based on approximations of the above fields, in the orientation space, by finite series of the generalized spherical harmonics. The algorithm of FEM analysis in this case is the same as that working under the Taylor assumption, but the number of degrees of freedom increases a few times.

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## Metoda elementów skończonych dla ośrodków z teksturą

Streszczenie

Sformułowanie teorii plastyczności kryształów niezależnej od prędkości deformacji, które korzysta z koncepcji powierzchni plastyczności o zaokrąglonych narożach, zostało zastosowane do analizy metodą elementów skończonych. Dla zadanej sieci elementów skończonych ośrodka makroskopowego i w małym otoczeniu każdego punktu całkowania rozpatrywana jest pewna liczba ziaren o budowie krystalicznej. Podejście takie umożliwia zarówno analizę sprężysto-plastycznego zachowania się materiału, na poziomie makroskopowym, jak i związanego z nim rozwoju tekstury oraz wzmocnienia systemów poślizgu, na poziomie mikroskopowym. Jednakże wymaga ono długiego czasu obliczeń spowodowanego dużą liczbą rozpatrywanych ziaren. Aby przyspieszyć obliczenia zamiast agregatu ziaren wprowadzono model kontinuum z teksturą.

W modelu tym wszystkie lokalne pola są ciąglymi funcjami sześciu zmiennych, które opisują położenie makroskopowego punktu oraz orientację mikroskopowej sieci krystalicznej. Algorytm MES jest taki sam jak dla modelu dyskretnego, ale liczba operacji numerycznych zmniejsza się około 50-krotnie. Model jest typu "fully constrained" tzn. że pracuje przy założeniu Taylora, kiedy lokalne pola odkształceń są takie same i pokrywają się z odkształceniem globalnym.

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