

PATRICK ZATTARIN*, ANDRZEJ BACZMAŃSKI**, PAWEŁ LIPIŃSKI**,
KRZYSZTOF WIERZBANOWSKI**

MODIFIED SELF CONSISTENT MODEL FOR TIME INDEPENDENT PLASTICITY OF POLYCRYSTALLINE MATERIAL

ZMODYFIKOWANY MODEL SAMOUZGODNIONY NIEZALEŻNEJ OD CZASU PLASTYCZNOŚCI MATERIAŁÓW POLIKRYSTALICZNYCH

Starting from the kinematics integral equation, which can be considered as a formal exact solution of the elasto-plastic homogenisation problem, a new version of the self consistent modelling is proposed. Three methods of active slip system selection are introduced and implemented in the self consistent code.

The predicted results as well as the calculation times are compared for different methods. The time of calculation strongly depends on the criterion used to select active systems. The ratio of five is found between the two extreme results. The developed model allows one to determine the overall elasto-plastic properties of the polycrystalline material but also the internal structure evolution described in the model by the grain shape, crystallographic lattice orientation, second order internal stresses and critical resolved shear stress for all slip systems.

Opracowano nową wersję modelu samouzgodnionego deformacji elasto-plastycznej, wychodząc z kinematycznego równania całkowego; to ostatnie uważane jest za dokładne rozwiązanie problemu homogenizacji elasto-plastycznej. Omówiono i przetestowano trzy metody wyboru aktywnych systemów poślizgu.

Rezultaty przewidywań modeli jak i czasy obliczeń są porównane dla wspomnianych trzech metod. Czas obliczeń zależy od użytego kryterium wyboru aktywnych systemów poślizgu i różni się o czynnik pięć pomiędzy dwoma skrajnymi wynikami. Opracowany model umożliwia przewidywanie globalnych własności elasto-plastycznych materiału polikrystalicznego, jak również ewolucji struktury wewnętrznej materiału, charakteryzowanej kształtem ziaren, orientacją sieci krystalicznej, naprężeniami wewnętrznymi drugiego rzędu oraz naprężeniami krytycznymi systemów poślizgu.

* LABORATOIRE DE PHYSIQUE ET MÉCANIQUE DES MATÉRIAUX, INSTITUT SUPÉRIEUR DE GÉNIE MÉCANIQUE, ILE DU SAULCY, 57045 METZ, CEDEX, FRANCE

** WYDZIAŁ FIZYKI I TECHNIKI JĄDROWEJ, AKADEMIA GÓRNICZO-HUTNICZA, 30-059 KRAKÓW, AL. MICKIEWICZA 30

NOTATION

The following conventions are used in this paper. Capital letters are applied to describe the overall (global) quantities, the lower cases correspond to the local variables and the "I" superscript is used for the averages for the I-th inclusion. Vectors and tensors are indicated by bold face symbols. The superimposed dot corresponds to time derivatives. The simple contraction of tensors is indicated with a single dot, the double dot corresponds to double contraction.

In this work the following notation is used:

A and A^I are the concentration tensors of velocity gradient,

$\mathbf{g}^I = \mathbf{g}^{Ie} + \mathbf{g}^{Ip}$ is the local velocity gradient for the I-th inclusion,

\mathbf{g}^{Ie} is its elastic part,

\mathbf{g}^{Ip} is its plastic part,

$\mathbf{G} = \mathbf{G}^e + \mathbf{G}^p$ describes the overall velocity gradient,

H^{sg} is the single crystal hardening matrix,

l and l^I correspond to the local tangent properties,

L is the overall tangent modulus tensor,

L^* is the Hill's constraint tensor,

m^g and n^g are the vectors describing slip systems,

$\dot{\mathbf{n}}$ is the rate of the local nominal stress tensor,

\dot{N} indicates the rate of the overall nominal stress tensor,

S^g is the Schmid's factor for g-th slip system,

T^{IJ} is the interaction tensor between the inclusions I and J ,

Γ is the modified Green tensor,

τ_{cr}^g defines the critical resolved shear stress for the g-th slip system.

1. Introduction

Since the pioneer work of Taylor [1], the modelling of plastic behaviour of polycrystalline materials has undergone an important evolution. One can cite for instance the approach proposed by Sachs [2] or the family of models based on the Taylor's idea with various modifications concerning the relaxation of some components of the stress or strain tensors, see for example [3, 4]. Excepting the crystallographic texture of the material, all these models neglect the granular structure of the polycrystal. A new way was opened by Kröner [5]. He was the first who introduced in mechanics (elasticity) a self consistent modelling of the inhomogeneous material properties. Hill [6] proposed an extension of this concept to the elasto-plasticity. The development of the self consistent approach is closely related to the fundamental work of Eshelby [7] concerning the description of interactions between an ellipsoidal inclusion and surrounding matrix. This solution allows one to take into account in modelling the evolution of the polycrystal grain shape and orientation.

The first applications of the self consistent scheme have been done by Budiansky and Wu [8], Hutchinson [9, 10] and Berveiller and Zaoui [11] in the framework of small elastoplastic strain theory. Iwakuma and Nemato-Nasser [12] have proposed an extension of the Hill's self consistent

scheme to the case of finite elasto-plastic transformations and they applied the obtained model to the 2D situations. The more systematic and general approach, based on the kinematic integral equation, has been developed by Lipiński and Berveiller [13] and Lipiński [14] and successfully applied for the 3D representative volume element under any large transformation loading path [15, 16]. Parallely, Wierzbowski [17] has proposed an original version of the Hill's model using Berveiller and Zaoui [11, 18] approximation of the plastic accommodation phenomenon.

The extensive use of the self consistent modelling, for instance as a particular constitute law included to Finite Element calculations, is restricted by an important time consumption when dealing with this method. The time is spent particularly on the choice of active slip systems and calculation of interaction tensors. The significant improvement of the last point has been accomplished by Zattarin, Lipiński and Carmasol [19]. The choice of active slip systems during a given load increment has remained an open and difficult question, especially in case of Taylor type modelling, for which the ambiguous combinations of slip systems frequently arrive.

In this paper we discuss and compare three various methods of the active slip system choice. The first one has been proposed and implemented by Lipiński [14] in his original self consistent code. The second one has been developed by Baczmański [20, 21] and results from the common experience of the French and Polish teams. The last one initially has been proposed by Leffers [22, 23] and next improved and intensively used by Wierzbowski et al. [17, 24, 25].

The present paper is divided into four parts. The next paragraph gives a brief description of the slip system theory. Paragraph 3 recalls the basic equations of the self consistent modelling, necessary to introduce the mentioned above three methods of slip system choice. This problem is presented in paragraph 4. In the last part we compare some results such as stress-strain curves, residual stresses, crystallographic textures, obtained using the three methods of slip system selection. The calculation times are also compared in this section.

2. Physical basis of the plasticity of metals at low temperature

Today, it is commonly admitted that the plastic flow of metals at low temperature is due to the dislocation motion. In 1958, Kröner [26] proposed the continuum theory of dislocations based on the dislocation density tensor introduced earlier by Nye [27]. Unfortunately, the continuum theory of dislocations is not developed enough to describe the behaviour of a single crystal. Some tentative of this kind of modelling have been done for instance by Kubin and Canova [28] showing the importance of this approach but their direct application to the polycrystal description still seems to be unrealisable.

Up till now the way which is habitually used corresponds to some kind of phenomenological homogenisation of the single crystal plastic flow. The theory is based on experimental observations of an important mobility of dislocations on surfaces commonly called *slip systems*. Outside of slip systems this mobility is practically unobservable. These slip systems are geometrically well defined for instance by Miller indices $[uvw](hkl)$ and they can be described by two unit vectors \mathbf{n}^s and \mathbf{m}^s . The vector \mathbf{n}^s is normal to the slip plane and vector \mathbf{m}^s indicates the slip direction. The external product of these two vectors is called the Schmid's factor \mathbf{S}^s . It plays an important role in the description of the single crystal plasticity

$$\mathbf{S}^s = \mathbf{m}^s \otimes \mathbf{n}^s. \quad (1)$$

The dislocations' motion produces, on the meso or single crystal scale, a relative, irreversible gliding of the material volumes separated by a slip "s". The rate of gliding is characterised by a scalar $\dot{\gamma}^s$. It can be shown that the kinematics of the plastic deformation is described by the linear combination of individual glides on the active slip systems

$$\mathbf{g}^p = \sum_{s=1}^{\text{NAS}} \mathbf{S}^s \dot{\gamma}^s, \quad (2)$$

where \mathbf{g}^p is the plastic part of the velocity gradient tensor and NAS states for Number of Active Systems. On the other hand, if one accepts the idea of Schmid, the plastic gliding can take place only when the resolved shear stress on the system "s".

$$\tau^s = (\boldsymbol{\sigma} \cdot \mathbf{n}^s) \cdot \mathbf{m}^s = \boldsymbol{\sigma} : \mathbf{S}^s \quad (3)$$

reaches some critical value τ_{cr}^s depending on the strain hardening state or dislocations arrangement in the single crystal, i.e.,

$$\tau^s \leq \tau_{cr}^s, \quad (4)$$

where $\boldsymbol{\sigma}$ in expression (3) is the Cauchy measure of the stress tensor. Let us assume that in the case of homogeneous multislip theory, i.e. when the spatial dislocations arrangement is not very pronounced, the hardening of the single crystal can be described by a hardening matrix \mathbf{H} reflecting the interactions among dislocations on slip systems, such that

$$\dot{\tau}_{cr}^s = \sum_{g=1}^{\text{NAS}} H^{sg} \dot{\gamma}^g. \quad (5)$$

In practice, the interaction between two slip systems, say g and s (where at least one is supposed to be active) depends on the dislocation density and the relative orientations of slip systems. Consequently they can be divided with some approximation into two groups [29, 17].

a) the weak hardening interactions, represented by the H_w term in the hardening matrix, correspond to:

- self hardening of the active system itself,
- the interaction of coplanar systems,
- the cross-slip system interactions,
- the interaction between systems with perpendicular slip directions,

b) the strong hardening interactions, represented by H_S term, correspond to the remaining slip system configurations.

Taking into account the above remarks, we can conclude that the hardening matrix can be constructed using two independent parameters, i.e. H_w and the hardening anisotropy factor $A = H_S/H_w$.

In this work the linear hardening i.e., constant H -matrix was assumed. Using the self consistent model (described below) one can predict the evolution of dislocation density ρ (where: $\rho \sim \tau_{cr}^2$) during elasto-plastic deformation. For a small equivalent strain i.e., $E_{eq} < 0.8$ the theoretical results show a very good agreement with the experimental ones obtained by analysis of the diffraction peak broadening. However for a large deformation the hardening matrix has to be modified in order to predict non-linear behaviour of the material [30]. In spite of the relatively rough approximations used to describe the single crystal behaviour, the above relations, when applied in the frame-work of scale transition theories, allow to predict complex material behaviours observed under experimental conditions corresponding to the presented restrictions, i.e. low temperature testing and homogeneous multislip deformation mechanism.

3. The self consistent (SC) modelling

The idea of the scale transition theory is used to study the material on at least two levels of observation. In case of polycrystalline materials these levels correspond to the single crystal (meso) scale and the global (macro) or representative volume element (RVE) scale. Let us suppose that the introduced below stress and strain measures are conjugated in the sense defined by Hill [6]. Later a particular choice of these measures will be proposed.

At the macroscopic level, we introduce the overall stress tensor Σ and strain tensor E (or their rates $\dot{\Sigma}$ and \dot{E}) characterising the external loading and material response. At the same time a polycrystalline grain “feels” the local stress $\sigma(\mathbf{r})$ or stress rate $\dot{\sigma}(\mathbf{r})$ and undergoes the local compatible strain $\varepsilon(\mathbf{r})$ or strain rate $\dot{\varepsilon}(\mathbf{r})$. The theory is based on the hypotheses of existence of a concentration tensor $A(\mathbf{r})$ such that, for example

$$\dot{\varepsilon}(\mathbf{r}) = A(\mathbf{r}) : \dot{E} \quad (6)$$

If the external loading is large enough to start the plastic deformation, the mechanical behaviour of the RVE can be described by the elastic E^e and plastic E^p parts which, in general, depend on the internal structure of the material. In the case of a plastically deformed crystallite, the corresponding elastic and plastic parts are

denoted by $\boldsymbol{\varepsilon}^e(\mathbf{r})$ and $\boldsymbol{\varepsilon}^p(\mathbf{r})$ or their rates. Supposing that we are able to describe the local behaviour of the material by the tangent elasto-plastic tensor $\mathbf{I}(\mathbf{r})$ such that

$$\dot{\boldsymbol{\sigma}}(\mathbf{r}) = \mathbf{I}(\mathbf{r}) : \dot{\boldsymbol{\varepsilon}}(\mathbf{r}) \quad (7)$$

the global effective properties \mathbf{L}^{eff} of the homogeneous equivalent material are given by

$$\mathbf{L}^{eff} = \frac{1}{V} \int_V \mathbf{I}(\mathbf{r}) : \mathbf{A}(\mathbf{r}) dV, \quad (8)$$

where V is the volume of the RVE. The main improvement of the self consistent approach, when compared with Taylor type modelling, is taking into account the interactions between a constituent and the surrounding material. This could be accomplished especially using the Eshelby [7] solution of the ellipsoidal inclusion problem. It implies that the shape of constituents in the self consistent approach is approximated by an ellipsoidal volume with the appropriate aspect ratio and spatial orientation with respect, for instance, to the crystal lattice and to the sample co-ordinates system.

During plastic deformation of constituents, the following physical phenomena influence the mechanical behaviour of the grain (see [16] and [17]).

- multiplication and annihilation of dislocations and evolution of their spatial distribution inside grains which lead to the hardening of the slip systems described by the evolution of critical resolved shear stresses,
- generation of the internal stresses by plastic incompatibilities,
- rotation of the crystal lattice of grains leading to a texture formation,
- modification of the grain shape and orientation.

To predict the accurate overall response of the material it is necessary to follow the evolution of grain parameters occurring during the slip and/or twinning phenomena. In the presented models only the first one, i.e. slip, is taken into account. As it has been demonstrated by Lipiński and Berveiller [13] the evolution of most of the above parameters is related to the local velocity gradient $\mathbf{g}(\mathbf{r})$. It can be shown that the nominal stress rate (see for instance [6]) is conjugated with the velocity gradient. The study of large elasto-plastic transformations of heterogeneous materials can be performed using updated Lagrangian formulation. All details of the modelling can be found in the work of Lipiński [14]. Here we only recall the fundamental results.

Let us suppose that the local elasto-plastic behaviour of single crystals can be expressed by the relation

$$\dot{\boldsymbol{\sigma}}(\mathbf{r}) = \mathbf{I}(\mathbf{r}) : \mathbf{g}(\mathbf{r}), \quad (9)$$

where $\dot{\boldsymbol{\sigma}}$ is the rate of the nominal stress tensor and $\mathbf{I}(\mathbf{r})$, as above, corresponds to the tangent properties of the material. Starting from the equilibrium equation and

supposing kinematic boundary conditions for RVE one can find the integral equation being the formal solution of our problem

$$\mathbf{g}(\mathbf{r}) = \mathbf{G}^0 - \int_V \mathbf{\Gamma}(\mathbf{r}, \mathbf{r}') : \delta \mathbf{l}(\mathbf{r}') : \mathbf{g}(\mathbf{r}') dV, \quad (10)$$

where:

\mathbf{G}^0 is the velocity gradient of a fictitious homogeneous material with properties \mathbf{L}^0 ,

$\delta \mathbf{l}(\mathbf{r}) = \mathbf{l}(\mathbf{r}) - \mathbf{L}^0$ is the deviation of local properties from \mathbf{L}^0 ,

$\mathbf{\Gamma}(\mathbf{r}, \mathbf{r}')$ is so called modified Green tensor.

To obtain the self consistent approximation of equation (10) we have to introduce two supplementary simplifications:

- we suppose the material is granular and the real grain shape can be approached by an ellipsoid,
- the tangent properties as well as the velocity gradient variations are very smooth inside grains, so their mean values \mathbf{l}^I and \mathbf{g}^I remain good approximations of the real behaviour.

Under these assumptions we can write

$$\mathbf{l}(\mathbf{r}) = \sum_{I=1}^N \mathbf{l}^I \theta^I(\mathbf{r}) \quad \mathbf{g}(\mathbf{r}) = \sum_{I=1}^N \mathbf{g}^I \theta^I(\mathbf{r}) \quad \text{and} \quad \delta \mathbf{l}(\mathbf{r}) = \sum_{I=1}^N \Delta \mathbf{l}^I \theta^I(\mathbf{r}),$$

where N is the number of constituents and

$$\theta^I(\mathbf{r}) = \begin{cases} 1 & \forall \mathbf{r} \in V_I, \\ 0 & \forall \mathbf{r} \notin V_I, \end{cases}$$

where V_I is the constituent volume. Finally, the integral equation (10) takes the form

$$\mathbf{g}^I = \mathbf{G}^0 - \sum_{J=1}^N \mathbf{T}^{IJ} : \Delta \mathbf{l}^J : \mathbf{g}^J. \quad (11)$$

This solution corresponds to so called “multi-site” approximation of the integral equation. This name is due to the presence of the tensor \mathbf{T}^{IJ} which describes the interactions between the I and J constituents. The interaction tensor is defined by the following expression

$$\mathbf{T}^{IJ} = \frac{1}{V_I} \int_{V_I} \int_{V_I} \mathbf{\Gamma}(\mathbf{r}, \mathbf{r}') dV' dV \quad (12)$$

It is easy to understand (but much more difficult to prove, see for example [26]), that if the homogeneous reference material is replaced by the effective unknown properties, i. e., if

$$\mathbf{L}^0 = \mathbf{L}^{eff} \quad (13)$$

then the long distance interactions given by T^{IJ} (with $I \neq J$) can be neglected in comparison with short distance interactions described by the tensor T^{II} . In this case one obtains the “one-site” self consistent approximation of integral equation (10)

$$\mathbf{g}^I = \mathbf{G} - T^{II} : \Delta I^I : \mathbf{g}^I \quad (14)$$

in which \mathbf{G}^0 has been replaced by \mathbf{G} , the true velocity gradient applied on the RVE boundary. This result may be transformed into the concentration relation

$$\mathbf{g}^I = (\mathbf{I} + T^{II} : \Delta I^I)^{-1} : \mathbf{G} = \mathbf{A}^I : \mathbf{G} \quad (15)$$

and next the self consistent approximation of the effective properties of the polycrystal can be calculated

$$\mathbf{L}^{sc} = \sum_{I=1}^N f^I \mathbf{A}^I \quad (16)$$

with f^I representing the volume fraction of I-th constituent and N being the number of grains. The simplicity of (14) comparing with expression (11) is only apparent because the relation (14) is implicit in character. Indeed, to calculate \mathbf{g}^I one needs to know $\mathbf{L}^{eff} \approx \mathbf{L}^{sc}$ which can be calculated knowing all \mathbf{g}^I or \mathbf{A}^I .

Of course the equation (14) may be rewritten as [6, 12] (see Appendix):

$$\dot{\mathbf{N}} - \dot{\mathbf{n}}^I = -\mathbf{L}^* : (\mathbf{G} - \mathbf{g}^I), \quad (17)$$

where

$$\mathbf{L}^* = (T^{II})^{-1} - \mathbf{L}^{sc} \quad (18)$$

is the so called Hill's constraint tensor.

Finally, let us transform relation (17) to the form similar to that used by Leffers [22, 23] and Wierzbanski et al. [24, 25]. The details of the transformation can be found in Appendix. We admit the additive decomposition of the velocity gradient into elastic and plastic parts following the relation

$$\mathbf{g}^I = \mathbf{g}^{Ie} + \mathbf{g}^{Ip} \quad (19)$$

than the Hill relation can be expressed as follows (see equations A7)

$$\dot{\mathbf{n}}^I = \mathbf{U}^I : \dot{\mathbf{N}} - \boldsymbol{\lambda}^I : \mathbf{g}^{Ip}, \quad (20)$$

where

$$\boldsymbol{\lambda}^I = \{s^I + (\mathbf{L}^*)^{-1}\}^{-1}, \quad (21)$$

$$\mathbf{U}^I = \boldsymbol{\lambda}^I : \{(\mathbf{L})^{-1} + (\mathbf{L}^*)^{-1}\} \quad (22)$$

and s^I expresses the grain elastic compliance tensor, see for instance [31]. One can easily observe that the λ^I and U^I tensors remain the same for all grains when the elastic properties of RVE are homogeneous. Expression (20) constitutes a new self consistent formulation of the polycrystalline plasticity, particularly well adapted for application of the *Leffers - Wierzbanski* [22, 24] method of active slip systems selection. Expression (14) constitutes a starting point for *Lipiński's* [14] and *Baczmanski's* [20, 21] algorithms of the active slip system choice.

4. Different methods of slip system selection

An incremental formulation of the above results has been developed for their numerical implementation. Suppose that at the end of step ($i-1$) all local and global variables describing the polycrystal are known. Particularly we suppose that new form and orientation of grains and their crystal lattices are updated and the self consistent approximation of tangent moduli is determined. At the step i the new increment of external loading is applied, i.e. the increment ΔN or ΔG is specified. Knowing L^{sc} and the shape and orientation of all grains one can calculate the interaction tensor T^{II} . The following procedures depend on the method of active slip system selection.

4.1. Minimal work criterion

According to the work of *Lipiński* [14] the active slip systems for the I -th grain are selected as follows:

1. knowing the local and global polycrystal properties at the end of step ($i-1$), the local stress tensor σ^I is updated,

2. the Schmid's criterion (3) is verified for all slip systems. Systems exceeding this criterion are called "potentially active". If NPAS means the number of such systems, one can construct 2^{NPAS} combinations of these systems (purely elastic response, corresponding to a local unloading, is included). For each combination we calculate:

a) the local tangent moduli I^I , concentration tensor A^I and velocity gradient g^I (see for instance *Lipiński* [14] and equation (15)),

b) the total strain energy of grain. The appropriate expression has been done by *Fassi-Fehri* [32] for the case of small strain approximations,

c) the combination with minimal strain energy is kept,

3. the combination having minimal strain energy is used to calculate the local tangent properties for the i -th step. Consequently, the local stress and strain, the grain lattice orientation and the critical resolved shear stress for each slip system are updated.

It is easy to understand that this approach requires many calculations. Indeed, for the advanced plastic flow $g^{Ip} > 0.015$) the number of potentially active systems is

frequently greater than 5. It means that frequently more than 32 complete constructions of local behaviour of each grain are necessary.

4.2. Maximal loading criterion

This criterion results from our experience concerning use of the scale transition methods. It appears that, except the elastic unloading case, the combination of active systems almost always corresponds to the most loaded systems, i.e. to the systems which exceed the most the Schmid's criterion. If one remembers that the plastic strain rate tensor has five independent components, one can, like for Taylor type models, restrict the number of active slip systems to the linearly independent ones. This method has been proposed and used by Baczmański [20, 21]. The flow chart of the first method is only slightly modified. The point 1 remains unchanged and point 2 becomes:

2. the Schmid's criterion (3) is checked for all slip systems. Systems exceeding this criterion are classified in increasing order with respect to the value of difference $\tau^s - \tau_{cr}^s$ (see also equations 3 and 4) and all linearly dependent systems are eliminated. It is possible to find out at maximum five mostly loaded and independent slip systems and these are supposed to be active ones if the strain energy corresponding to this solution is less than that of the purely elastic response,

3. as before, the chosen combination is used to calculate the local tangent properties and to update the local stress and strain states, the grain lattice orientation and the critical resolved shear stress for each slip system.

4.3. Leffers-Wierzbanski criterion

This approach has been used by Leffers [22] and later by Wierzbanski [17, 24, 25] in Berveiller and Zaoui [18] type of modelling based on *a priori* estimated isotropic constraint tensor L^* . Their idea can be shortly summarised as follows. Only one, the most loaded, slip system is active for a very short time. During this time (subincrement) a small amount of shear glide $\delta\gamma^s$ occurs. This glide produces an increment of plastic velocity gradient, which causes a modification of the stress state, critical resolved stresses and lattice orientation of a given grain. If these modifications are important enough and if more than one slip system should be active for a given loading increment, another system becomes the most loaded and the procedure is repeated until there is no system exceeding the Schmid's criterion. The only difficulty which arises when dealing with this method is the estimation of the tangent properties of the single crystal. To resolve this problem, one has to count the instantaneously active systems and at the end of loading increment the linearly independent combination has to be determined. The application of this method is based on formula (20) where the local stress evolution is

directly linked with the plastic part of velocity gradient \mathbf{g}^{Ip} . The following procedure explains the practical use of this method.

1. Knowing the L^{sc} tensor for the $i-1$ step the interaction tensor T^{II} and constraint tensor L^* are determined by (12) and (18).

2. The local stress state σ^I is updated using (20) and supposing a purely elastic response of the single crystal.

3. The Schmid's criterion (3) is checked for all slip systems.

4. The most loaded system (i.e., with maximum difference $\tau^s - \tau_{cr}^s$) is chosen among all potentially active systems:

a) the elementary glide of amplitude $\delta\gamma^s$ is realised on this system producing some $\delta\mathbf{g}^{Ip}$,

b) the local stress state σ^I is modified together with the internal structure of the grain,

c) the number of active slip system is stored,

d) the Schmid's criterion (3) is verified for all slip systems.

5. If there are systems exceeding Schmid's criterion return to point 4.

6. The combination of active systems is build and the single crystal tangent properties are calculated.

Whatever the method of the system selection, the loading increment is completed by calculations of the effective properties of the RVE. This is accomplished using equation (8). The global stress and strain state are determined by the averaging operations. We recall that the strain averaging can be performed only for the total strain E . The elastic part of strain tensor E^e can be calculated using the inverse Hooke's law and the decomposition rule of the total strain on elastic and plastic part permits to calculate E^p .

5. Comparison of different methods of active slip systems selection

The above developed approaches have been applied to predict the elasto-plastic behaviour of different materials, namely BCC, FCC and hexagonal structure polycrystals. We have simulated a cold rolling process using a RVE samples represented by 2500 grains having initial random crystallographic orientations defined with respect to the macroscopic frame by three Euler angles ϕ_1 , Φ , and ϕ_2 . All slip systems of all grains have the same critical resolved shear stress. The initial grain shape is supposed to be spherical. Finally, the volume fraction is chosen identical for all grains and equal to $f^I = 0.0004$. For FCC and BCC structures we have considered an isotropic elastic response of the material, however, for the hexagonal symmetry anisotropic elastic constants were assumed for each grain. The hardening matrix is isotropic and the linear hardening law is considered (i.e. linear relationship between critical resolved shear rate and rate of gliding). All micro-parameters necessary to perform the simulations are given in the table 1.

Input parameters describing initial microstructure of materials

Structure (grain shape)	Slip systems (total number)	τ_{cr} — critical resolved stress [Mpa]	Hardening matrix [Mpa]	Elastic constants for the grain [GPa]
BCC (spherical)	$\langle 111 \rangle \{110\}$ $\langle 111 \rangle \{112\}$ $\langle 111 \rangle \{123\}$ (48 glides)	82	$H_w = 60$ $A = 1$	$\mu = 80$ $\lambda = 120$
FCC (spherical)	$\langle 110 \rangle \{111\}$ (12 glides)	100	$H_w = 100$ $A = 1$	$\mu = 45.5$ $\lambda = 96.8$
Hexagonal (spherical)	$\langle 2110 \rangle \{0001\}$ $\langle 2110 \rangle \{0110\}$ $\langle 2110 \rangle \{0111\}$ (12 glides)	100	$H_w = 100$ $A = 1$	$C_{11} = 160$ $C_{33} = 181$ $C_{44} = 46$ $C_{12} = 90$ $C_{13} = 66$

As one can see the introduced properties correspond to:

- typical ferritic steel (BCC material),
- copper (FCC material),
- titanium alloy (hexagonal material).

Nine simulations have been performed using three criteria for the slip system elimination:

1. *the minimum energy or work criterion (MW),*
2. *the maximum load criterion (ML),*
3. *Leffers-Wierzbanski criterion (LW).*

Figure 1 presents equivalent stress-strain curves obtained for three materials using three criteria of slip system selection. The equivalent stress and strain are defined in the sense of von Mises. For all the curves, one can observe the experimentally well established behaviour which can be decomposed on:

- first stage, until 0.03 to 0.05 of equivalent strain, with parabolic evolution due to the progressive activity of slip systems, see for comparison figure 2 and 3. This stage corresponds to the activation of the second order internal stresses which guarantee the compatibility of deformation of the individual grains.

- second stage ($E_{eq} > 0.05$) with a quasi constant slope, function of the hardening parameter and number of active slip. To obtain the non-linear material behaviour one has to introduce a non-linear hardening relation for the single crystal, see for instance [29].

One can observe that some differences exist for stress-strain curves obtained using the three criteria. Especially for LW criterion the equivalent stress is slightly lower.

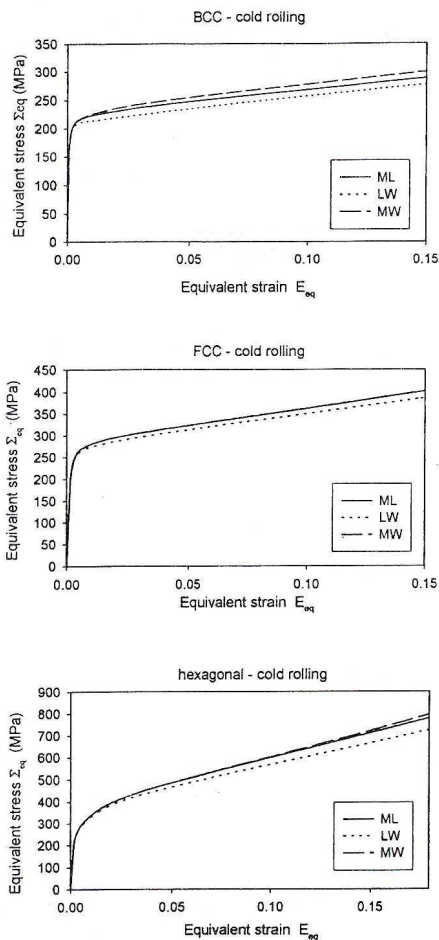


Fig. 1. Equivalent applied stress Σ_{eq} vs. equivalent strain E_{eq} obtained by different criteria of slip systems selection for BCC, FCC and hexagonal structures

Fig. 2 shows the evolution of the tangent modulus in rolling direction as a function of the equivalent total strain. This modulus is defined as the inverse of the 1111 component of the inverted L -matrix of the overall material properties (i.e., $E_T = 1/(\mathbf{L}^{-1})_{1111}$). One can observe that this modulus becomes quasi constant for the equivalent strain greater than 0.05. Its „asymptotic” value is:

$$\begin{aligned}
 E_T &\approx 600 \text{ MPa for BCC material,} \\
 E_T &\approx 1000 \text{ MPa for FCC polycrystal,} \\
 E_T &\approx 2200 \text{ MPa for hexagonal structure.}
 \end{aligned}$$

The three methods of slip system selection predict practically the same evolution of this modulus.

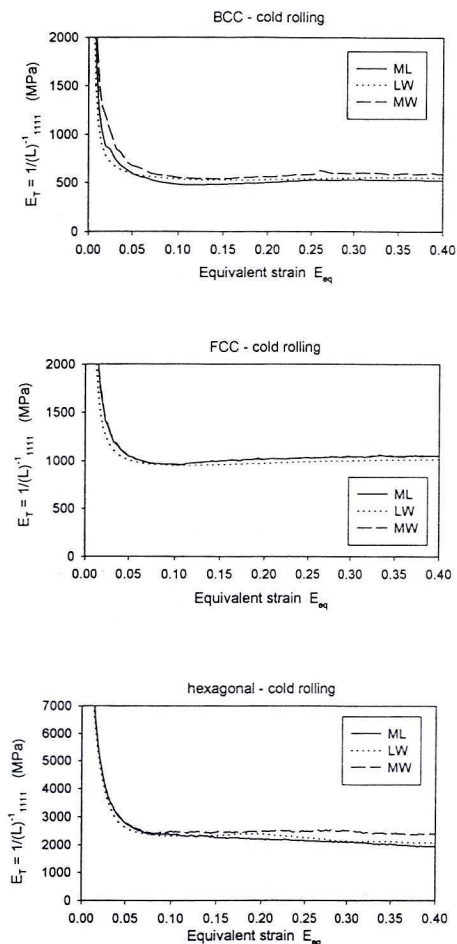


Fig. 2. Evolution of the tangent modulus $E_T = 1/(L^{-1})_{1111}$ vs. equivalent E_{eq} for different criteria and structures

The slip system activation statistics are shown in Fig. 3. The mean number of instantaneously active systems for an arbitrary grain is presented as a function of the equivalent total strain. We see that for BCC, FCC and hexagonal polycrystal about three systems are permanently active for $E_{eq} \geq 0.05$. Once again, one can conclude that the three methods predict almost the same responses.

The crystallographic textures induced by the rolling operation are presented by cross sections through the basic part of the Euler space (Fig. 4). The Orientation Distribution Function (ODF) obtained numerically for $E_{eq} = 0.6$ of equivalent plastic strain are compared with the experimental ones. The textures were measured using neutron method on the 6T1 diffractometer at Orphee reactor (LLB, CEA-CE, Saclay, France). One can see a very good agreement between theoretical and experimental results. The three criteria proposed in this work give practically the

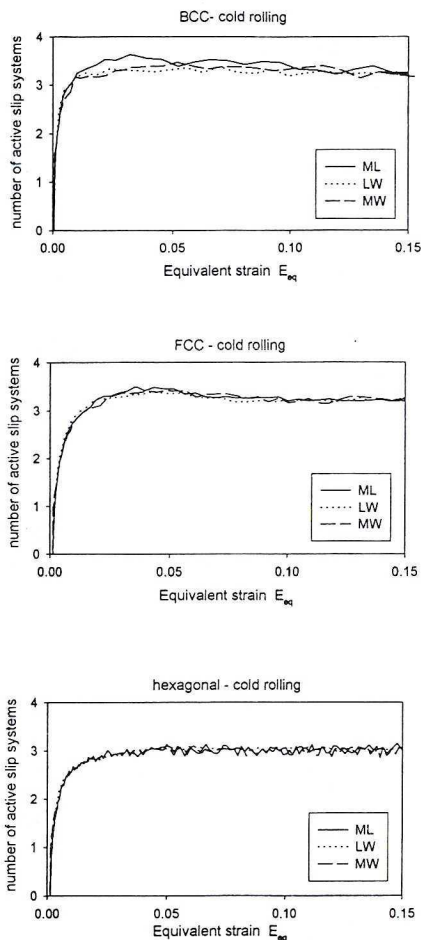
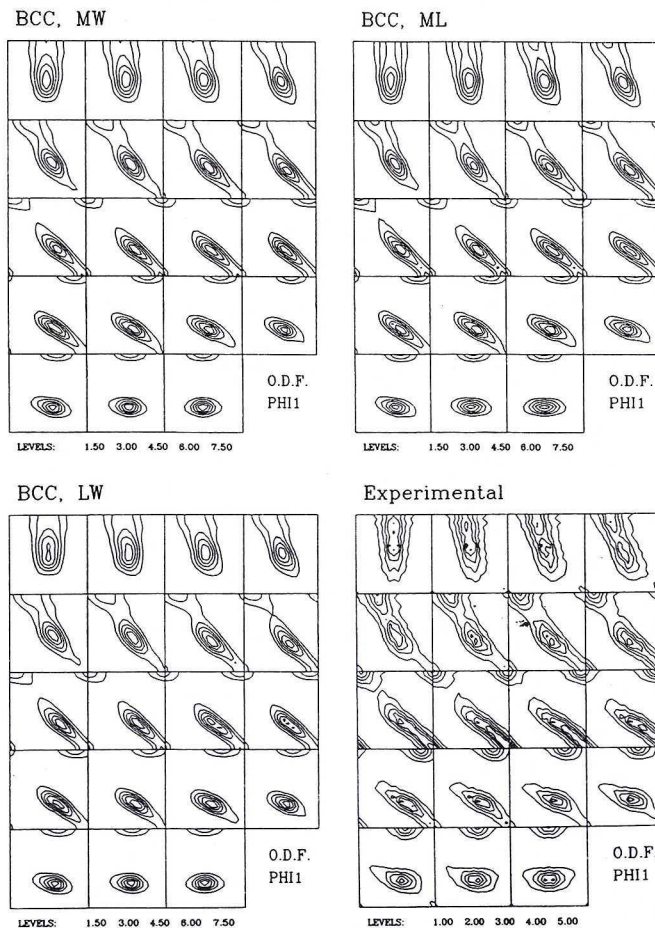


Fig. 3. The mean number of active slip system for one grain of polycrystal. Comparison for different criteria of slip system selection

same ODFs for the FCC, BCC and hexagonal (not shown in Fig. 4) structures. (It is important to note, that two characteristic types of texture exist in FCC materials: the copper and brass types. The presented self consistent model predicts only the first one, i.e., the copper type texture, because of its very precisely determined — and rather hard — interaction between a grain and its neighbourhood. The brass type texture can be obtained if the interaction intensity is lowered; it is the case of models developed by Leffers [22] and by Wierzbanski et al. [17, 24, 25]).

The last comparison is made for BCC structure only. Fig. 5 shows the effect of the plastic strain history on residual second order stresses. After plastic deformation the shape of a crystallite does not fit, in general, to the surrounding matrix (plastic strain differs from one grain to another). Hence, the grains are subjected to elastic strain caused by incompatibilities in their boundary regions. This creates the so called

a)



second order residual stresses which are „frozen” in the material. Additionally, in the real sample some residual macrostresses arise because of deformation heterogeneity. For example the compressive macrostress can be found on the surface of the cold rolled sheet. All these residual stresses cause distortion of the crystallographic lattice which can be measured by diffraction methods.

Usually, the stress state is studied using the ε vs. $\sin^2(\psi)$ graphs, where ε is the measured lattice strain and ψ is the angle between scattering vector and direction normal to the sample. It can be shown that ε (strain) is linear with $\sin^2(\psi)$ for isotropic samples and residual macrostresses. The second order stresses can be observed as the nonlinearities in the ε vs. $\sin^2(\psi)$ plot.

In Fig. 5b the prediction of the self consistent model with maximal load (ML) criterion is compared with experimental measurements. The theoretical data were fitted to measured lattice strains [20, 21] and the values of residual macrostress $\sigma_{11} = -70.5$ MPa and microstress $\sigma_{eq} = 83.9$ MPa were found. One can see that the

b)

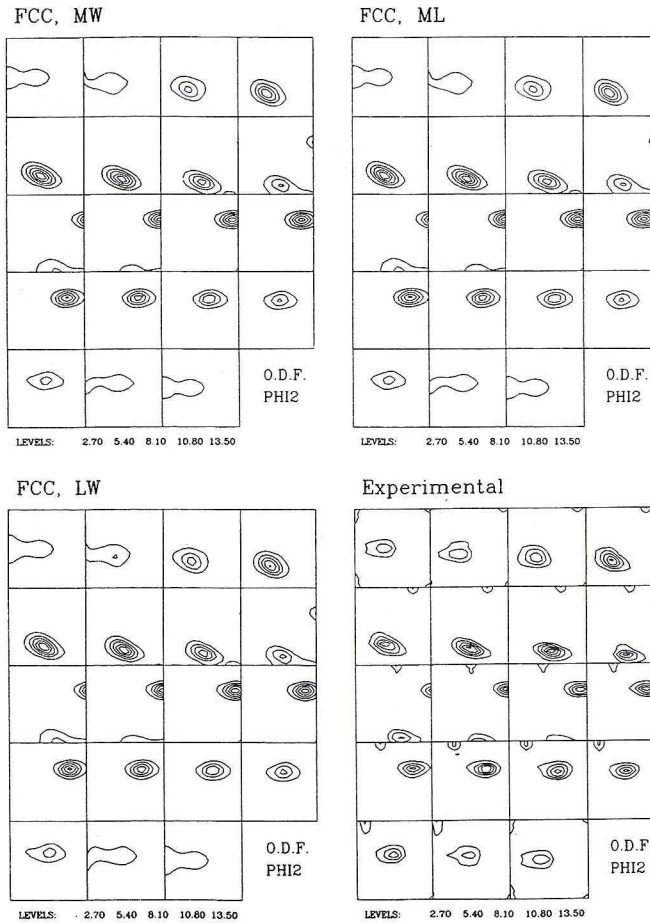


Fig. 4. Crystallographic texture for cold rolling deformation. Predicted Orientation Distribution Functions (for $E_{eq} = 60\%$) are compared with experimental ones ($E_{eq} = 105\%$ for BCC and $E_{eq} = 100\%$ for FCC structures)

variation of the second order strains (stresses) in function of the crystal orientation is well predicted. Probably, because of stress relaxation in the grain boundaries the calculated strains were about twice higher than the experimental ones. Hence, the theoretical strains shown in Fig. 5b were multiplied by the constant factor $q = 0.45$. The numerical results obtained using the three presented models are practically identical (see Fig. 5a).

As the last point, we compare the calculation times using different criteria for slip system selection. The results are shown in table 2. It can be seen that the time of calculations improves about 5 times if the new criteria for the slip system selection are used. In the case of LW criterion the time is shorter for elastically isotropic

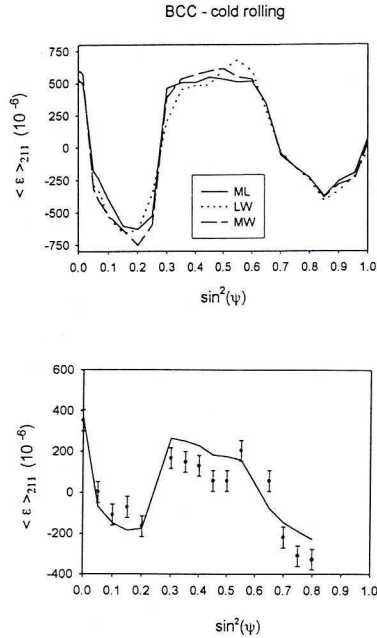


Fig. 5. Average lattice strain for (211) reflection vs. $\sin^2(\psi)$ (result for BCC is shown); where ψ is the angle between scattering vector and direction normal to the sample (scattering vector, rolling and normal directions are laying in the same plane): a) comparison for different criteria of slip systems selection, b) theoretical result based on the *maximum load* model (solid line) is fitted to experimental points

sample (BCC and FCC structures) than for the anisotropic one (hexagonal structure). It is due to the fact that the λ^I and U^I tensors in equations (20)–(22) remain the same for all elastically isotropic grains.

TABLE 2

Relative time of calculations for 2500 grains deformed to equivalent strain of 0.6. Isotropic elastic properties were assumed for FCC and BCC structures and anisotropic elastic constants were used for the hexagonal sample

Structure	MW criterion	ML criterion	LW criterion
BCC	1	0.28	0.20
FCC	0.81	0.16	0.17
Hexagonal	0.75	0.17	0.24

Conclusions

A new method for the prediction of elasto-plastic deformation of the polycrystalline materials has been proposed. This scheme is particularly well adapted to the Leffers and Wierzbanski algorithm of the active systems selection.

Three different methods for selection of active slips were tested and compared. In two of proposed methods the most loaded systems were taken as the active ones. In one case the independent most loaded systems are supposed to be simultaneously active. In the second case the elementary single slips are performed on most loaded system. The results of calculations are very similar to these obtained from the traditional model in which the minimum work criterion is used. It can be concluded, that the way of selection of active slips does not change much the model predictions. However, it is crucial for the calculation time. Using the presented methods our computer program has been accelerated approximately five times and potentially it can be used in the Finite Elements (FEM) calculations.

The model has been applied to predict the behaviour of FCC, BCC, and hexagonal materials. The predicted overall material response exhibits correct hardening curves. The comparison of the calculated and experimental crystallographic textures shows a very good agreement between the calculations and measurements. The same conclusion concerns the comparison between the predicted and measured residual stresses.

Acknowledgements

- A. Baczmański and K. Wierzbowski thank to:
 — Komitet Badań Naukowych (Polish Committee of Scientific Research) for financial support.
 — the LLB, CEA Saclay (France) for enabling them to use neutron diffraction.

APPENDIX

Derivation of the formulas used in the model based on LW criterion

As it has been stated in the paragraph 3, the concentration relation (15) can be transformed into Hill — Iwakuma and Nemat-Nasser expression (17). Let us recall the relation (15) in slightly modified form

$$[I + T^{II} : (I^I - L)] : g^I = G. \quad (A1)$$

After some simple transformations this relation can be rewritten as follows

$$[I^I - L + (T^{II})^{-1}] : g^I = [L - L + (T^{II})^{-1}] : G \quad (A2)$$

or using local and global constitutive relations

$$\dot{n}^I = \dot{N} + [(T^{II})^{-1} - L] : (G - g^I). \quad (A3)$$

This is the Iwakuma and Nemat-Nasser [12] expression (17) containing the Hill's constraint tensor

$$L^* = (T^{II})^{-1} - L. \quad (A4)$$

One can see that when dealing with homogeneous materials, i.e. when $\mathbf{l}^I = \mathbf{L}$ or $\Delta \mathbf{l}^I = 0$, all these expressions give the expected trivial response

$$\mathbf{g}^I = \mathbf{G} \quad \text{or} \quad \dot{\mathbf{n}}^I = \dot{\mathbf{N}}.$$

This occurs for cases of purely elastic response (initial loading or local or global unloading) of elastically homogeneous materials.

Now, let us return to equation (A3) and split the velocity gradient \mathbf{g}^I into the elastic (\mathbf{g}^{Ie}) and plastic (\mathbf{g}^{Ip}) parts

$$\dot{\mathbf{n}}^I = \dot{\mathbf{N}} + \mathbf{L}^* : (\mathbf{G} - \mathbf{g}^{Ip} - \mathbf{g}^{Ie}). \quad (\text{A5})$$

The elastic part of the velocity gradient can be calculated as a function of the local nominal stress rate

$$\mathbf{g}^{Ie} = \mathbf{s}^I : \dot{\mathbf{n}}^I$$

where \mathbf{s}^I describes the elastic behaviour of grains, see [31]. Introducing the above relation into (A5) and using the overall constitutive equation we obtain

$$(\mathbf{I} + \mathbf{L}^* : \mathbf{s}^I) : \dot{\mathbf{n}}^I = (\mathbf{I} + \mathbf{L}^* : \mathbf{L}^{-1}) : \dot{\mathbf{N}} - \mathbf{L}^* : \mathbf{g}^{Ip} \quad (\text{A6})$$

which can be transformed into

$$\dot{\mathbf{n}}^I = \mathbf{U}^I : \dot{\mathbf{N}} - \boldsymbol{\lambda}^I : \mathbf{g}^{Ip} \quad (\text{A7a})$$

or

$$\dot{\mathbf{n}}^I = \mathbf{A}^I : \mathbf{G} - \boldsymbol{\lambda}^I : \mathbf{g}^{Ip} \quad (\text{A7b})$$

where

$$\boldsymbol{\lambda}^I = \{\mathbf{s}^I + (\mathbf{L}^*)^{-1}\}^{-1}$$

$$\mathbf{U}^I = \boldsymbol{\lambda}^I : \{(\mathbf{L})^{-1} + (\mathbf{L}^*)^{-1}\}$$

and

$$\mathbf{A}^I = \mathbf{U}^I : \mathbf{L}.$$

Expressions (A7) are used respectively for boundary conditions (overall loading) of kinematic or static type.

REFERENCES

- [1] G. I. Taylor, Plastic strain in metals, *J. Inst. Metals* **62**, 307 (1938).
- [2] G. Sachs, Zur abteilung einer fleissbedingung, *Zeit. Der V.D.I.* **72**, 739 (1928).
- [3] P. Van Houtte, On the equivalence of the relaxed Taylor theory and the Bishop Hill theory for partially constrained plastic deformation of crystals, *Mat. Sci. Engng* **55**, 69 (1982).
- [4] G. R. Canova, C. N. Tome, U. F. Kocks, J. J. Jonas, The yield surface of textured polycrystals, *J. Mech., Phys. Solids* **33**, 371 (1985).

- [5] E. Kröner, Zur plastischen verformung des vielkristalls, *Acta Metall* **9**, 155 (1961).
- [6] R. Hill, Continuum micro-mechanics of elastoplastic polycrystals, *J. Mech. Phys. Solids* **13**, 89 (1965).
- [7] J. D. Eshelby, The determination of the elastic field of an ellipsoidal inclusion, and related problems, *Proc. Roy. Soc.* **A241**, 376 (1957).
- [8] B. Budiansky, T. T. Wu, Theoretical prediction of plastic strains of polycrystals, *Proc., 4th US Nat. Cong. of Applied Mech.*, 1175 (1962).
- [9] J. W. Hutchinson, Plastic stress-strain relations of FCC polycrystalline metals hardening according to Taylor rule, *J. Mech. Phys. Solids* **12**, 11 (1964).
- [10] J. W. Hutchinson, Plastic deformation of BCC polycrystals, *J. Mech. Phys. Solids* **12**, 25 (1964).
- [11] M. Berveiller, A. Zaoui, An extension of the self-consistent scheme to plastically flowing polycrystals, *J. Mech. Phys. Solids* **26**, 325 (1979).
- [12] T. Iwakuma, S. Nemat-Nasser, Finite elastic-plastic deformation of polycrystalline metals, *Proc. R. Soc. Lond.* **A394**, 87 (1984).
- [13] P. Lipiński, M. Berveiller, Elastoplasticity of micro-inhomogeneous metals at large strains, *Int. J. of Plasticity* **5**, 149 (1989).
- [14] P. Lipiński, Modélisation du comportement des métaux, en transformations élastoplastiques finies, à partir des méthodes de transition d'échelles, Habilitation, University of Metz (1993).
- [15] P. Lipiński, J. Krier, M. Berveiller, Elastoplasticité des métaux en grandes transformations: comportement global et évolution de la structure interne, *Rev. Phys. Appliquée* **25**, 361 (1990).
- [16] P. Lipiński, A. Naddari, M. Berveiller, Recent results concerning the modelling of polycrystalline plasticity at large strains, *Int. J. Solids Structures* **29**, 1873 (1992).
- [17] K. Wierzbowski, Some results of a theoretical study of plastic deformation and texture formation in polycrystals, *Scientific Bulletins of St. Staszic University of Mining and Metallurgy*, No 1132, *Phys. Bull.* **12** (1987).
- [18] M. Berveiller, A. Zaoui, Méthode self-consistente en mécanique des solides hétérogènes. 15^{ème} Colloque du Groupe Français de Rheologie, Paris, France, 175 (1980).
- [19] P. Zattarin, A. Carmasol, P. Lipiński, Une nouvelle approche numérique pour calculer les interactions entre deux inclusions dans un milieu anisotrope, *Compt. Rend. 3^{ème} congrès de mécanique, SMSM, Maroc*, 845 (1997).
- [20] A. Baczański, K. Wierzbowski, J. Tarasiuk, M. Ceretti, A. Lodini, Anisotropy of Micro-Stresses Measured by Diffraction, *Rev. de Metall.* **94**, 1467 (1997).
- [21] A. Baczański, K. Wierzbowski, J. Tarasiuk, Models of Plastic Deformation Used for Internal Stress Measurements, *Z. Metallkd.* **86**, 507 (1995).
- [22] T. Leffers, *Phys. Stat. Sol.* **25**, 337 (1968).
- [23] T. Leffers, A. Kinematic Model for the Plastic Deformation of Face-Centred Cubic Polycrystal Riso Report No 302, Danish Atomic Energy Commission, Riso, Denmark (1975).
- [24] K. Wierzbowski, Z. Jasieński, Some Comments on Sachs and Taylor Type Deformation, *Scripta Met* **15**, 585 (1981).
- [25] K. Wierzbowski, J. Jura, W. G. Haije, R. B. Helmholtz, FCC Rolling Texture Transitions in Relation to Constraint Relaxation, *Cryst. Res. Technol.* **27**, 513 (1992).
- [26] E. Kröner, *Kontinuumstheorie der Versetzungen and Eigenspannungen*, Berlin, Springer-Verlag (1958).
- [27] J. F. Nye, *Physical properties of crystals*, Clarendon, Press Oxford (1957).
- [28] L. P. Kubin, G. Canova, The modelling of dislocation patterns, *Scripta Metall Mater.* **27**, 957 (1992).
- [29] P. Franciosi, M. Berveiller, A. Zaoui, Latent hardening in copper and aluminium single crystals, *Acta Met* **28**, 273 (1980).
- [30] Ch. Schmitt, P. Lipiński, M. Berveiller, Micromechanical modelling of the elastoplastic behaviour of polycrystals containing precipitates. Application to hypo and hyper eutectoid steels, *Int. J. Plasticity* **13**, 183 (1997).

- [31] R. Hill, On the elasticity and stability of perfect crystals at finite strain, *Math. Proc. Camb. Phil. Soc.* **77**, 225 (1975).
- [32] O. Fassi-Fehri, Le problème de la paire d'inclusions plastiques et hétérogènes dans une matrice anisotrope, Ph. D. Thesis, University of Metz (1985).

REVIEWED BY: PROF. DR HAB. INŻ. ZDZISŁAW JASIEŃSKI

Received: 10 March 2000.