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General theory of isothermic elastic-plastic deformation of polycrystals.
[Preliminary communication]

PŘEDBĚŽNÁ SDĚLENÍ

GENERAL THEORY OF ISOTHERMIC ELASTIC – PLASTIC DEFORMATION OF POLYCRYSTALS [PRELIMINARY COMMUNICATION]

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The presented theory supposes the micro-stresses to be of essential importance for the variations of mechanical properties of polycrystals, caused by plastic deformation.

If a statistically homogeneous and isotropic material is considered, the following mathematical model seems to be proper:

The material is supposed to consist of N basic materials, which all are of Reuss' type, without strain-hardening, with Mises' criterion of yielding, with all parameters different. Further it is supposed, that the basic materials are dispersed in micro-volumes and on the contact-surfaces of the micro-volumes no displacements occur. It holds

$$(1) \qquad de_{ijn} = \mu_n \, ds_{ijn} \, ,$$

$$(2) \qquad d\varepsilon_n = \varrho_n \, d\sigma_n$$

in the elastic state and

$$(3) \qquad de_{ijn} = s_{ijn} \, d\lambda_n + \mu_n \, ds_{ijn} \, ,$$

$$(4) \qquad d\varepsilon_n = \varrho_n \, d\sigma_n \, ,$$

$$(5) \qquad s_{ijn} s_{ijn} = 2k_n^2$$

in the plastic state of the n-th basic material.

In the analysis that follows the above quantities with n-indices are considered as the arithmetical averages in the micro-volumes of the n-th material.

Then we can write

$$(6) \qquad \sum_{n=1}^{N} \vartheta_n \sigma_{ijn} = \bar{\sigma}_{ij} \, ,$$

$$(7) \qquad \sum_{n=1}^{N} \vartheta_n \varepsilon_{ijn} = \bar{\varepsilon}_{ij} ,$$

$$(8) \qquad \sum_{n=1}^{N} \vartheta_n = 1 .$$

The elastic potential of the average stresses is

$$(9) \qquad W = \sum_{n=1}^{N} \vartheta_n \left(\tfrac{3}{2} \varrho_n \sigma_n^2 + \tfrac{1}{2} \mu_n s_{ijn} s_{ijn} \right) .$$

This is of course not the whole potential energy in a macroscopic unit volume, as the arithmetic average is in general not identical with the quadratic one and then, from the Schwarz's inequality it follows, that the whole potential energy must be greater than (9).

The micro-volumes of the n-th material resist the average deformation ε_{ijn} and the difference between this proper deformation and the macroscopic deformation.

It is supposed, that the whole potential energy may be expressed approximately in the following way

$$(10) \qquad P = W + V = W + \xi \sum_{n=1}^{N} \vartheta_n \left(\tfrac{3}{2} \varrho_n \sigma_n'^2 + \tfrac{1}{2} \mu_n s_{ijn}' s_{ijn}' \right) ,$$

where

$$(11) \qquad \mathrm{d}\sigma_n' = \frac{\mathrm{d}\varepsilon_n - \mathrm{d}\bar{\varepsilon}}{\varrho_n} , \quad \mathrm{d}s_{ijn}' = \frac{\mathrm{d}e_{ijn} - \mathrm{d}\bar{e}_{ij}}{\mu_n}$$

in the elastic state.

Similarly if in the n-th material the plastic state is reached, the increment of the respective plastic work refered to macroscopic unit volume is

$$(12) \qquad \mathrm{d}D_n = \vartheta_n \left(2k_n^2 + \xi s_{ijn}' s_{ijn}' \right) \mathrm{d}\lambda_n .$$

At the elastic limit the quantity s_{ijn}' may be calculated according to the equation (11). Further increments of s_{ijn}' are

$$(13) \qquad \mathrm{d}s_{ijn}' = \frac{1}{\mu_n} \left(\mathrm{d}e_{ijn} - s_{ijn}' \, \mathrm{d}\lambda_n - \mathrm{d}\bar{e}_{ij} \right) .$$

The increment of the whole microscopic work is then

$$\mathrm{d}(W + V + D) .$$

The increment of the macroscopic work is

$$\mathrm{d}\Pi = \bar{\sigma}_{ij} \, \mathrm{d}\bar{\varepsilon}_{ij} .$$

All further necessary equations for the derivation of the stress-strain relations and their variations can be obtained from the generalized principle of the virtual work

$$(14) \qquad \delta(W + V + D - \Pi) = 0 \,.$$

As an example let us consider $N = 2$ and a pure shear loading $\bar{s}_{\alpha\beta}$. We shall suppose, that in the original state all the micro-stresses are zero with the only exception of $s_{\beta\gamma n} = s^0_{\beta\gamma n}$. (The deviatoric micro-stress-components seem to correspond to the oriented micro-stresses, observed in X-ray investigations.) According to (6) it must hold

$$(15) \qquad s^0_{\beta\gamma 2} = - \frac{\vartheta_1}{\vartheta_2} s^0_{\beta\gamma 1}$$

and from the above considerations it follows

$$(16) \qquad s'^0_{\beta\gamma 1} - s'^0_{\beta\gamma 2} = - \frac{s^0_{\beta\gamma 1}}{\vartheta_2 \xi} \,.$$

According to (6) it is valid in general

$$(17) \qquad s_{ij2} = \frac{1}{\vartheta_2} (\bar{s}_{ij} - \vartheta_1 s_{ij1}) \,,$$

$$(18) \qquad \sigma_2 = \frac{1}{\vartheta_2} (\bar{\sigma} - \vartheta_1 \sigma_1)$$

and in this way the variables are the macroscopis components and the components with the index 1.

In the elastic state we obtain from the equations (only two are independent)

$$(19) \qquad \frac{\partial(W + V - \Pi)}{\partial s_{\alpha\beta 1}} = \frac{\partial(W + V - \Pi)}{\partial s_{\beta\gamma 1}} = \frac{\partial(W + V - \Pi)}{\partial \bar{s}_{\alpha\beta}} = 0$$

the following results

$$(20) \quad s_{\alpha\beta 1} = \frac{\mu_2}{\vartheta_1\mu_2 + \vartheta_2\mu_1} \left[1 + \frac{\vartheta_2\mu_1(\mu_1 - \mu_2)}{\mu_1\mu_2 + \xi(\vartheta_1\mu_1 + \vartheta_2\mu_2)(\vartheta_1\mu_2 + \vartheta_2\mu_1)} \right] \bar{s}_{\alpha\beta} =$$

$$= \frac{\mu_1\mu_2 + \xi(\vartheta_1\mu_1 + \vartheta_2\mu_2)\mu_2}{\mu_1\mu_2 + \xi(\vartheta_1\mu_1 + \vartheta_2\mu_2)(\vartheta_1\mu_2 + \vartheta_2\mu_1)} \bar{s}_{\alpha\beta} \,,$$

$$(21) \qquad s_{\beta\gamma 1} = s^0_{\beta\gamma 1} \,.$$

The equivalent expressions (20) show, that the value of $s_{\alpha\beta 1}$ lies between analogous values of $s_{\alpha\beta 1}$ calculated from the supposition $s_{ijn} = \bar{s}_{ij}$ and the supposition $e_{ijn} = \bar{e}_{ij}$ which gives $s_{\alpha\beta 1} = \mu_2/(\vartheta_1\mu_2 + \vartheta_2\mu_1) \bar{s}_{\alpha\beta}$.

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It can be easily shown that the equation (20) is general, holding for arbitrary loading in elastic state and for arbitrary deviatoric component, when $s_{\alpha\beta 1}^0 = 0$. When not, then (20) holds for $(s_{\alpha\beta 1} - s_{\alpha\beta 1}^0)$.

Analogously it can be derived

$$(22) \quad (\sigma_1 - \sigma_1^0) = \frac{\varrho_2}{\vartheta_1\varrho_2 + \vartheta_2\varrho_1} \left[1 + \frac{\vartheta_2\varrho_1(\varrho_1 - \varrho_2)}{\varrho_1\varrho_2 + \xi(\vartheta_1\varrho_1 + \vartheta_2\varrho_2)(\vartheta_1\varrho_2 + \vartheta_2\varrho_1)} \right] \bar{\sigma} =$$

$$= \frac{\varrho_1 + \xi(\vartheta_1\varrho_1 + \vartheta_2\varrho_2)}{\varrho_1\varrho_2 + \xi(\vartheta_1\varrho_1 + \vartheta_2\varrho_2)(\vartheta_1\varrho_2 + \vartheta_2\varrho_1)} \varrho_2\bar{\sigma} \, .$$

Let us consider now, that in the material 1 and only in the material 1 the plastic limit has been reached. Then it holds

$$(23) \qquad\qquad s_{\alpha\beta 1}^2 + s_{\beta\gamma 1}^2 = k_1^2 \, ,$$

$$(24) \qquad\qquad ds_{\beta\gamma 1} = - \frac{s_{\alpha\beta 1}}{s_{\beta\gamma 1}} ds_{\alpha\beta 1} \, .$$

From the above considerations and from the following equations (from which only two are independent)

$$(25) \quad \frac{\partial(W + V + D - \Pi)}{\partial s_{\alpha\beta 1}} = \frac{\partial(W + V + D - \Pi)}{\partial \lambda_1} = \frac{\partial(W + V + D - \Pi)}{\partial \bar{s}_{\alpha\beta}} = 0$$

it can be calculated

$$(26) \qquad d\lambda_1 = \frac{\mu_2[\mu_1 + \xi(\vartheta_1\mu_1 + \vartheta_2\mu_2)] s_{\alpha\beta 1}}{\xi\vartheta_2[(\vartheta_1\mu_1 + \vartheta_2\mu_2) k_1^2 - \mu_2(s_{\alpha\beta 1}s_{\alpha\beta 1}' + s_{\beta\gamma 1}s_{\beta\gamma 1}')]} d\bar{s}_{\alpha\beta} \, ,$$

$$(27) \quad ds_{\alpha\beta 1} = \frac{\mu_2[\mu_1 + \xi(\vartheta_1\mu_1 + \vartheta_2\mu_2)] [(\vartheta_1\mu_1 + \vartheta_2\mu_2) s_{\beta\gamma 1} - \mu_2 s_{\beta\gamma 1}'] s_{\beta\gamma 1}}{[\mu_1\mu_2 + \xi(\vartheta_1\mu_1 + \vartheta_2\mu_2)(\vartheta_1\mu_2 + \vartheta_2\mu_1)] \, .} \, d\bar{s}_{\alpha\beta} \, ,$$
$$\cdot \, [(\vartheta_1\mu_1 + \vartheta_2\mu_2) k_1^2 - \mu_2(s_{\alpha\beta 1}s_{\alpha\beta 1}' + s_{\beta\gamma 1}s_{\beta\gamma 1}')]$$

$$(28) \qquad d\bar{e}_{\alpha\beta} = d\bar{\varepsilon}_{\alpha\beta} = \vartheta_1\mu_1 \, ds_{\alpha\beta 1} + \vartheta_1 s_{\alpha\beta 1} \, d\lambda_1 + \vartheta_2\mu_2 \, ds_{\alpha\beta 2} =$$

$$= \left\{ \bar{\mu} + \frac{\vartheta_1\mu_2^2[\mu_1 + \xi(\vartheta_1\mu_1 + \vartheta_2\mu_2)] \, .}{\xi\vartheta_2[\mu_1\mu_2 + \xi(\vartheta_1\mu_1 + \vartheta_2\mu_2)(\vartheta_1\mu_2 + \vartheta_2\mu_1)] \, .} \right\} d\bar{s}_{\alpha\beta} \, ,$$
$$\cdot \frac{\{[\mu_1 + \xi(\vartheta_1\mu_1 + \vartheta_2\mu_2)] s_{\alpha\beta 1} + \xi\vartheta_2(\mu_1 - \mu_2) s_{\alpha\beta 1}'\} s_{\alpha\beta 1}}{\cdot [(\vartheta_1\mu_1 + \vartheta_2\mu_2) k_1^2 - \mu_2(s_{\alpha\beta 1}s_{\alpha\beta 1}' + s_{\beta\gamma 1}s_{\beta\gamma 1}')]}$$

where

$$(29) \qquad\qquad \bar{\mu} = \frac{(1 + \xi)\,\mu_1\mu_2(\vartheta_1\mu_1 + \vartheta_2\mu_2)}{\mu_1\mu_2 + \xi(\vartheta_1\mu_1 + \vartheta_2\mu_2)(\vartheta_1\mu_2 + \vartheta_2\mu_1)}$$

is the macroscopic value of μ.

The preliminary calculations and comparison with experimental results have shown a very good possibility of description of the elastic-plastic behaviour of polycrystals by this mathematical model already when considering $N = 2$.

<div align="center">NOMENCLATURE</div>

$\sigma_{ijn}, \varepsilon_{ijn}, s_{ijn}, e_{ijn}$	stress- and strain-tensor components and respective deviatoric components in the n-th material,
$\bar{\sigma}_{ij}, \bar{\varepsilon}_{ij}, \bar{s}_{ij}, \bar{e}_{ij}$	respective macroscopic values,
σ	$= \frac{1}{3}\sigma_{ii}$,
ε	$= \frac{1}{3}\varepsilon_{ii}$,
E	modulus of elasticity,
ν	Poisson's ratio,
i, j, k	indices that can equal 1, 2, 3 and by repetition the summation is to be understood,
α, β, γ	indices that can equal 1, 2, 3, by repetition no summation is to be understood and $\alpha \neq \beta \neq \gamma \neq \alpha$,
n	index that can equal 1, 2, ..., N and by repetition no summation is to be understood,
μ	$= (1 + \nu)/E$,
ϱ	$= (1 - 2\nu)/E$,
$d\lambda_n$	parameter of the plastic deformation in the n-th material,
k_n	plastic limit of the n-th material if loaded by pure shear,
ϑ_n	volume fraction of the n-th material,
ξ	parameter depending on the structure of the material.

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