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MODELLING OF ELASTIC-PLASTIC DEFORMATION OF POLYCRYSTALLINE AND COMPOSITE MATERIALS UNDER LOADING

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Abstract- The process of deformation development in a polycrystal with grain interaction is modelled in frames of flat two-dimensional elastic-plastic flow of the media with structure. The processes of a possible fragmentation and a grain boundary segregation influence on the plastic deformations development are considered. The influence of distribution of a work under non-elastic deformation on material structure change and average value of mechanical parameters determination is analising in the presented calculations of deformation of a composite material with damping matrix .

1. Method of numerical modeling.

Let us write down the full equation system of the elastic-plastic deformation of the media on a mesoscopic level according to /1/ for the flat flow for which:

$\bar{u} = \{ u_1, u_2, 0 \}$; $\bar{\omega} = \{ 0 , 0 , \omega_3 \}$.

The deformed state is defined by

$$\dot{\gamma}_{ji} = \dot{u}_{i,j} - \varepsilon_{kij}\dot{\omega}_k \; ; \quad \dot{\ae}_{ji} = \dot{\omega}_{i,j} \; . \qquad (1)$$

The mass conservation law:

$$\partial\rho/\partial t + \rho\dot{u}_{i,i} = 0 \quad , \quad (i = 1,2) \quad . \qquad (2)$$

The equations of motion:

$$\sigma_{ji,j} = \rho\ddot{u}_i \; ; \quad \varepsilon_{ijk}\sigma_{jk} + \mu_{ji,j} = J\,\ddot{\omega}_i \quad , \qquad (3)$$

where ε_{ijk} - Levi-Civita tensor; J - measure of rotary inertia of a

particle ; $\bar{\omega} = \{\omega_i\}$ - rotation vector of a particle; $\bar{u} = \{u_i\}$ - displacement vector, the comma means differentiation on space coordinates and the point means time differentiation.
The constitutive equations:

$$\dot{\sigma}_{ij} = \lambda(\dot{\gamma}^{T}_{kk} - \dot{\gamma}^{p}_{kk})\delta_{ij} + (\mu + \alpha)(\dot{\gamma}^{T}_{ij} - \dot{\gamma}^{p}_{ij}) + + (\mu - \alpha)(\dot{\gamma}^{T}_{ji} - \dot{\gamma}^{p}_{ji}) \quad ;$$

$$\dot{\mu}_{ij} = \beta(\dot{æ}^{T}_{kk} - \dot{æ}^{p}_{kk})\delta_{ij} + (\nu + \varepsilon)(\dot{æ}^{T}_{ij} - \dot{æ}^{p}_{ij}) + + (\nu - \varepsilon)(\dot{æ}^{T}_{ji} - \dot{æ}^{p}_{ji}) \quad . \tag{4}$$

Here $\dot{\gamma}^{T}_{kk} = \dot{\gamma}^{e}_{kk} = \dot{\gamma}^{e}_{11} + \dot{\gamma}^{e}_{22}$, $\dot{\gamma}^{p}_{kk} = 0$, according to the plastic incompressibility postulate, $\dot{æ}^{T}_{kk} - \dot{æ}^{p}_{kk} = 0$ for flat flow.

Let us write down the energy conservation law not taking into account a heat conduction and an internal heat generation

$$\rho\dot{E} = \sigma_{ij}\dot{\gamma}_{ij} + \mu_{ij}\dot{æ}_{ij} \quad . \tag{5}$$

The system of equations (1)÷(5) was being solved numerically by the finite element method, that had been modified for dynamic problems /2/. A plastic behaviour of the medium was described by reducing a stress state to the yield circle. As $\sigma_{12} \neq \sigma_{21}$, when the second invariant of the stressed state was being calculated the corresponding term was being taken by $1/2(\sigma_{12} + \sigma_{21})$.

It is possible to use the relaxation form of the constitutive equation (4) when solving two-dimensional problems with taking account of structural element interactions, but it demands using of fine grids because of small real relaxation times. So it is difficult to realize practically such using because of insufficient capacity of computers. This problem was discussed in details in /3/, the model calculations were presented.

2. Modeling of a polycrystalline specimen deformation.

For imitating of the behaviour of the polycrystal with chaotic located grains the parameters of strong aluminum alloy D-16 were used. The specimen with initial configuration shown on fig.1.a was extended with some constant rate (sufficiently large for saving computer time). It was considered for simplicity that the resistance to the plastic shear of monocrystalline grains may be characterized by a scalar quantity - tentative yield strength σ_{Ti}. which were various for various grains (i - number of grain). The shear strength σ_{TTi} of a close to boundary region (is shown in fig.1 by dotted lines) was taken different from the grain shear strength. Cases with less strong and more strong close to boundary regions were examined.

Elastic modules α, ν, ε appear in the constitutive equations (4). Those parameters were taken of variable values in numerical experiments. The magnitude of α was 10% of shear module μ in results shown in fig.1. The order of magnitude ($\nu + \varepsilon$) was estimated from the consideration that couple-stresses $\mu \cong \tau \cdot l$, where l is a fragment size, and rotations of the fragments are about several degrees but usually less than 10÷20° according to the experiments /4/.

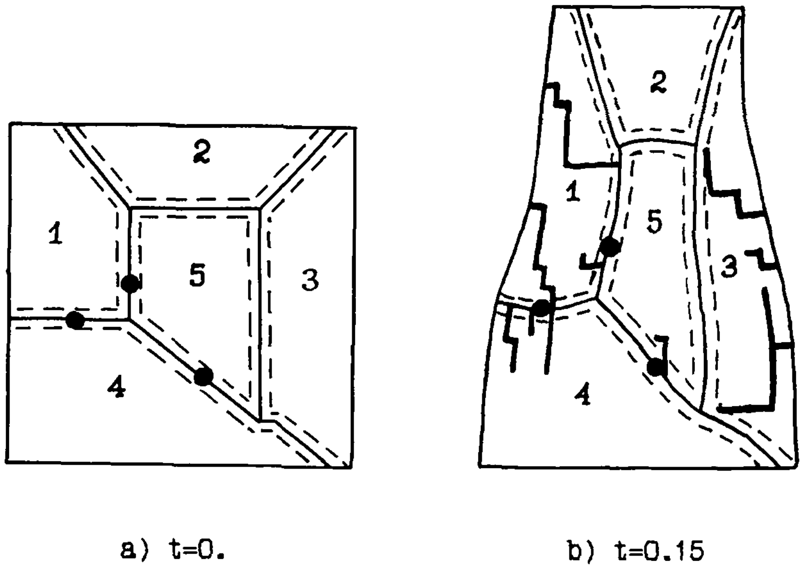


Fig.1. Numerical modeling of deformation of a polycrystalline specimen. Here t is undimensional time.

Heterogeneities of structure are the sources of couple-stresses and bending-torsion appearance. That is why the through method of calculation is applied, in accordance with which calculation of rotations, bend-torsions and couple-stresses in all the calculated grid elements is envisaged. The heterogeneity of shear strength results in rotation of certain sections of calculated grid relative to others, with resulting in bend-torsion and couple-stresses appearance. The space steps in numerical solution Δx_1 and Δx_2 are the characteristic sizes in realized approach, so the inertia momentum J in (3) is to be determined for an elementary calculated cell with the characteristic size Δx_i. The rotation of the hole grain make its appearance integrally. The medium within the grain being homogeneous and change of properties (σ_{Ti} of grain, σ_T of segregated firm phases, σ_{TTi} of close to boundary regions) taking place only on boundaries crossing, maximum couple-stresses and bend-torsion appear just on the boundaries. Such a through computation allows to take into account a possible fragmentation within a grain.

Plastic shears regions form shear bands which is shown in fig.1 by thick lines. In our computations the shear bands were determined as the place with a maximum gradient of the work under plastic deformation for each grain separately (as shear strength of grains are different). In shear bands work under plastic deformation essentially (several times sometimes) increase the work in next to ranges. In such bands one can determine new boundaries if proper criterions are generated and form more fine fragments by such a way.

In fig.1 the results for less strength close to boundary regions is presented. The concrete values of the tentative yield strength were : σ_{T1}= 0.1 GPa, σ_{T2}= 0.08 GPa, σ_{T3}= 0.25 GPa, σ_{T4}=0.2 GPa, σ_{T5}= 0.3 GPa. It was assumed that shear strength of close to boundary regions σ_{TTi} for each grain were 75÷80% of corresponding value of σ_{Ti}. The black circles on fig.1 denote firm inclusions, their strength being much grater than σ_{Ti}. The inclusions generated only small shears except the one in boundary of 1 and 4 grains. It is interesting that the shears in grain 1 from this inclusion and from a specimen boundary propagate to meet each other. The joints of grains (1,2,5) and (2,3,5) were stress concentrators here.

3. Modeling of composite material deformation.

The analogous approach has been applied to modeling of deformation processes of composite materials. Some ceramics with damping matrix has been considered: ZrO_2 matrix with Al_2O_3 inclusions and NiTi matrix with TiC inclusions. Typical fragment of such ceramics structure is shown in fig.2. The strain diagram of the matrix is shown in fig.3, its form to be determined by the martensite transformation within the deformation range.

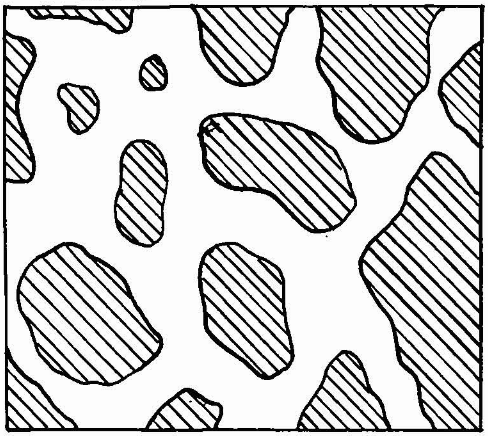


Fig. 2. Typical structure of composite NiTi + TiC.

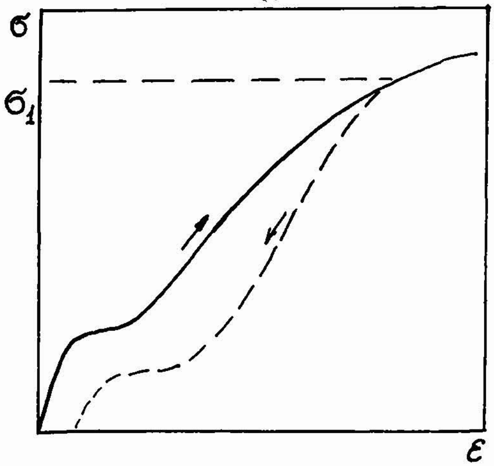
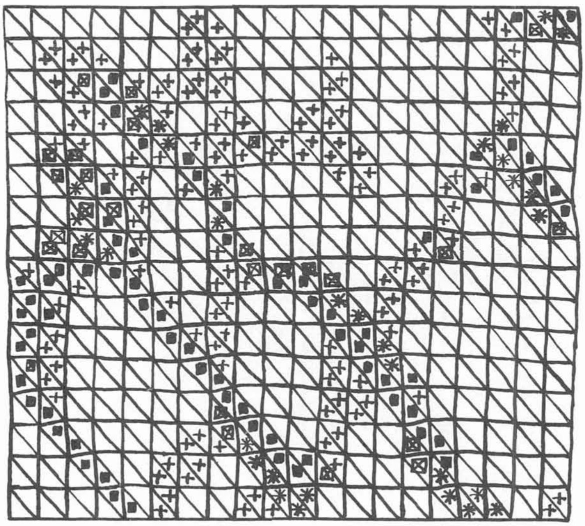


Fig. 3. A strain diagram of the material with martensite transformation.

The results of elastic-plastic analysis of fragments shown in fig. 2 is presented in fig.4. The mark ▪ indicates the binder zones with limiting value of the work done under non-elastic deformation.



Marked cells denote the regions with values of non-elastic work W:

▪ – $0.75W_p < W < W_p$;

* – $0.5W_p < W < 0.75W_p$;

⊠ – $0.25W_p < W < 0.5W_p$;

\+ – $0 < W < 0.25W_p$,

where W_p is the limiting value of W.

Fig. 4 Analysis of deformation of a composite material.

This zones determine prefracture regions and the boundaries of new fragments to be formed. Those values of work corresponds to σ_1 level in the strain diagram (fig.3). The accommodation effects appearance and as the result the formation of new mesostructure is caused by new boundaries appearance. The analysis of structure fragments deformation energy variation in the loading process allows us to estimate the average value of mechanical parameters and the contribution of different mechanisms of plastic deformation in them.

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