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NUMERICAL MODELING OF PLASTIC-SHEAR GENERATION AND EVOLUTION IN CRYSTALS UNDER LOADING

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Abstract

In early works we have proposed an approach to numerical modeling of elastoplastic deformation in crystals, taking into account plastic shear appearance near surface and interface and step-by-step propagation into the crystal volume. In this paper we continue to develop this approach as applied to simulation of both repeat generation of plastic shears by surface and interface sources and plasticity in polycrystal with slip planes.

Keywords: numerical modeling, mesomechanics, heterogeneous structures, surface and interface effects

1. Introduction

In our early works [1-5], a new approach to the numerical simulation of the elastoplastic behavior of solids under load, which combines mathematical modeling and a simulation technique, was outlined. In order to take into account the processes occurring at the mesolevel, use was made of a model including the effects of interfaces and those of the specimen's free surface on initiation and propagation of bands of localized plastic deformation. The numerical procedure involves application of the finite-difference method [6] from continuum mechanics and certain discrete-modeling techniques [7]. In the cited procedure, each of the cells of the finite-difference computational grid is considered to be a cellular automaton in an elastic or plastic state depending on the stress and strain experienced by this cell and its nearest neighbors. A plasticity criterion for an individual cell is formulated on the basis of experimental evidence for the nucleation of plastic shears at the surface and interfaces. This technique allows plastic flow in different elastoplastic media to be adequately simulated [1-5].

In this work, the foregoing approach is further developed as applied to the simulation of meso and macroscale plastic deformation in crystals. We treat plastic deformation as a repeat process of plastic shear generation by internal boundaries and surface and plastic flow propagation into the volume in step-by-step mode. Another advance of the model is simulation of plastic deformation in the polycrystal with including into consideration slip planes.

2. Mathematical approach

A system of differential equations of continuum mechanics, including the conservation laws [6] and the constitutive equations in a relaxation form [2], completed by initial and boundary conditions is numerically solved by the finite-difference method [6]. According to this method, area under calculation is marked by a computational grid with rectangular cells, and the differential equations given for a continuous medium are substituted by the finite-difference analogs defined for cells and nodes of the computational grid.

A main feature of the approach we proposed in [1-5] is concerned with a formulation of yield criterion taking into account surface and interface effects.

Experimental data [8-11] indicate that dislocations initially existing in crystals are fixed and does not make a contribution to plastic deformation. Under continuous loading movable dislocations originate at the free surface and internal boundaries, forming bands of localized plastic deformation, which propagate as plastic fronts from sources into material volume. To describe these processes we developed a numerical procedure, according to which, each cell of the calculation grid is considered as a cellular automaton that can be either in elastic or plastic state. Plastic deformation initially developed on the surface and at interfaces is translated from cell to cell in a step-by-step fashion.

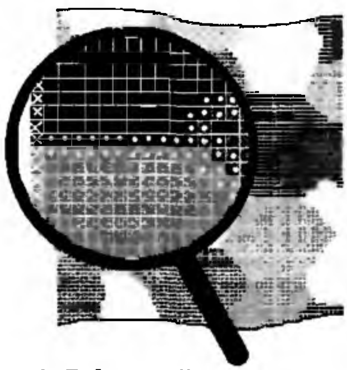

Figure 1: *Polycrystalline testpiece marked by computational grid. Computational cells varied in color are of different mechanical characteristics; x-marked are the surface cells; dot-marked are the interface cells.*

For the processes to be numerically described, every cell of the computational grid must “feel” not only what structure component it refers to, but its location in testpiece and state of nearest cells as well. For so doing, we developed an algorithm that controls elastoplastic behavior of any computational cell, taking into account stress-strain state and location of this cell and its neighbors as well. Among all the computational cells covering the structure component we marked those located at the surface and interfaces, fig. 1, and permitted for plastic shears to be nucleated there. Some critical values for the computational cell are the threshold stress triggering plastic deformation in it and the threshold built-up plastic strain responsible for translating the plastic shear from this cell to neighboring ones. The computational cell placed *inside* the structure element can be involved into plastic deformation by flow *coming from* the surface or/and interface. Thus, plastic shears propagate progressively into the crystal from surface/interface nucleation sources.

It should be noted that the character of *localized-deformation propagation* is controlled by the criteria of the plastic-shear translation assumed in the model. By selecting material-specific criteria, one can simulate different modes of plastic deformation development.

3. Simulation of repeat generation of plastic shears by surface and interface sources

According to experimental evidence [8, 9], first plastic shears nucleate in surface grains under external stresses about 10^5 times lower than the theoretical strength. As loading continues, a portion of surface grains plastically deformed increases and at certain critical level of external stresses plastic deformation begins to translate into material volume. The dislocation flow, propagating from the surface source and involving elastically deformed regions into plastic yielding, results in local stress relaxation. As external loading continues, stress applied to surface sources increases and once it reaches the critical value, the next portion of dislocations starts to move as a front of localized plastic deformation from the source into the crystal volume. Under continuous loading this process periodically repeats.

To simulate numerically this process in [4] we have made an advance of the yield criterion developed in [1]. Let us consider an act of plastic shear translation by the example of *i*-th cell. It is assumed that plastic shears in the *i*-th cell build up until a critical value of plastic strain has been reached. Then plastic shears translate to the neighboring cell(s) and plastic deformation of the *i*-th cell stops to develop until the next plastic shears has come to it from a source. Experimental data [8-11] indicate that an important condition for plastic deformation to propagate is presence of stress and dislocation density gradients. In this connection we formulate a criterion of plastic yielding as following: a material local area (computational cell) is able to become plastic, provided that stress and strain gradients between it and neighboring particle(s) have reached the critical values.

Together with the elastic constants, we introduce into consideration the limit of relaxation σ_r, up to which the stress can relax under the active load. We assumed for this value to be constant for all cells independently on their position in the calculation area. Parameters, which depend on the cell position in calculation area, are the stress of plastic shear generation σ_g the „excessive" plastic deformation ε^* and the effective stress gradient σ^*.

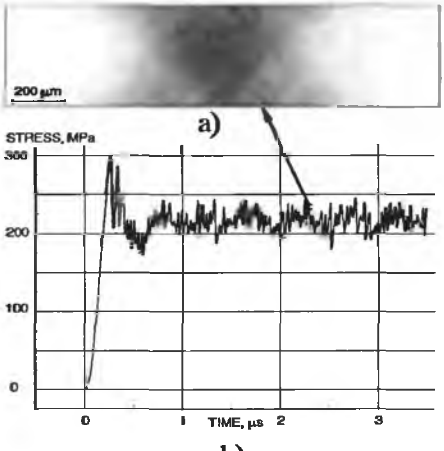

Figure 2: *Plastic deformation pattern (a) and time-dependent average stress (b) calculated from the model of repeat generation of plastic shears*

Calculation results presented in this section were performed for a macroscopic testpiece subjected to tension at strain rate about 10^2/s. Elastic modules, density and constants for barotropic equation of state correspond to the characteristics of aluminum alloy Al6061-T6 [2]. Interfaces were not included into consideration and surfaces of the testpiece served as sources of plastic shears. Values of the critical parameters were preset as follows: $\varepsilon^*=0.1\%$, $\sigma_g=\sigma_r=30$ MPa, $\sigma^*=300$ MPa. In this case the critical values of excessive strain and stress gradient are the basic parameters, which determine the nature of elastic-plastic behavior.

As boundary condition we set on the both opposite sides of test pieces particle velocities, which correspond to strain rate of 10^2/s (Fig. 2a). These sides could freely move in the direction perpendicular to the tension. Conditions on the other two boundaries imitated free surfaces. Such a formulation of boundary conditions excepts influence of the grips as macroscopic stress concentrators.

Plastic shears originated simultaneously on both opposite surfaces, approximately in the middle of the area under calculation. As external load increases, localized shear bands begin to propagate into the testpiece volume perpendicular to tension direction. The bands move in a pulse fashion controlled by both defect generation by surface sources and heterogeneous stress-strain state due to an interaction between elastically and plastically deformed regions. Such a behavior results in serrations in time-dependent stress integrated over the computational area, fig. 2b. The first peak of highest amplitude corresponds to formation and propagation of the first band of localized plastic deformation. The high level of stresses is attributed to stress increasing in local regions elastically deformed. That, in turn, leads to increasing in both stress gradients through the shear band fronts and value of the excessive plastic strain. Thus, as plastic deformation propagates into the testpiece volume, the criterion of plastic shear translation more easily fulfills that leads to increasing in speed of shear band propagation. As a result there is an intensive stress relaxation on the time-dependant stress curve, Fig. 2b.

Under continuous loading, plastic deformation covers all the cross-section and then localizes (fig. 2a). However, generation and propagation of plastic shears continue to affect the shape of stress-strain curve. It is interesting to note that a curve, which could be circumscribed about peaks of the time-dependent stresses in fig. 2b, is the pulse-shaped either. Period of the pulses approximately corresponds to time of shear band propagation through the testpiece cross-section, starting from its generation by the surface source.

4. Simulation of plastic deformation in polycrystal with considering for slip planes

In this section we present another advance of the model [1-5] as applied to simulation of plastic deformation in polycrystalline material with including into consideration slip planes. In this case the yield criterion controls not only plastic shear appearance and development in local areas but also their translation in certain direction. It is evident that in general case of polycrystalline material containing a reach variety of slip planes arbitrary oriented it is necessary to introduce into the model a tensor of critical parameters. That is the critical values of stresses and plastic strains will depend on slip plane orientation relative to direction of external loading.

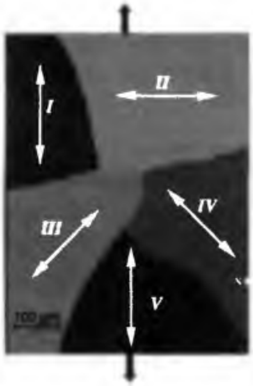

Figure 3: *Polycrystalline testpiece with slip planes.*

In this paper we simulate a simplest case of several grains (fig. 3), every of which has the only slip plane oriented at 0° (*I* and *V* grains), 90°(*II* grain) and 45°(*III* and *IV*) to load direction. According to the basic model [1], plastic shears can nucleate at the intergrain boundaries and then translate from the boundary sources into the grains. Direction of plastic shear propagation is preset for each of grains by a special numerical procedure simulating slip planes.

Computational results presented in fig. 4 as patterns of plastic strain rate, plastic deformation and velocity vectors demonstrate formation of mesoscale band of localized plastic deformation in the testpiece (fig. 3).

The patterns of plastic strain rates (fig. 4a) indicate that at the initial stage of loading plastic shears appear along all the intergrain boundaries, and this plastic deformation is localized in character. Local areas exhibiting intensive plastic deformation alternate with those, in which plastic strain rate is equal to zero. The reason is that plastic shears appearing in local zones of grain boundary result in stress relaxation, which partially unload neighboring areas elastically deformed.

Under continuous loading the plastic shears begin to propagate from the boundary sources into grain volumes in directions preset (refer to fig. 3). Note that character of plastic shear development is mainly controlled by macroscopic loading conditions. Individual plastic shears propagating from different boundary sources in preset directions, form, as a result, a mesoscale band of localized plastic deformation, orientation of which coincides with a vector of maximum tangential stresses.

Grain *II*, in which plastic shears could be only translated perpendicular to the vector of external force, remains elastically deformed. It is interesting to mark that other grains more favorably oriented to the load direction are not entirely involved into the plastic yielding. That is an evolution of individual plastic shears is mainly focused on generation of the mesoscopic band. Once the meso band of localized plastic deformation has formed, further plastic yielding localizes there.

A correlation between velocity fields (fig. 4c) and plastic deformation patterns (fig. 4b) has revealed some interesting phenomena relative to evolution of intergrain boundaries. Pay attention to the grain *I* located in top of the crystal, fig. 3. At the initial stage of loading plastic shears propagate from the upper boundary parallel to tension direction and form a narrow band of localized plastic deformation, separating the grain into two parts, which further behave themselves as individual grains. Similar pattern is observed as mesoscopic shear band forms and separates the grain *III* into two parts shearing each to other under continues loading. We believe that such processes are similar to appearance of new intergrain boundaries.

It is interesting to consider features of plastic yielding near interface between grains *III* and *V*. Plastic shears generated by the boundary are translated from the interface sources as a front of plastic deformation. As the front propagates into the grain *V*, the intergrain boundary stops

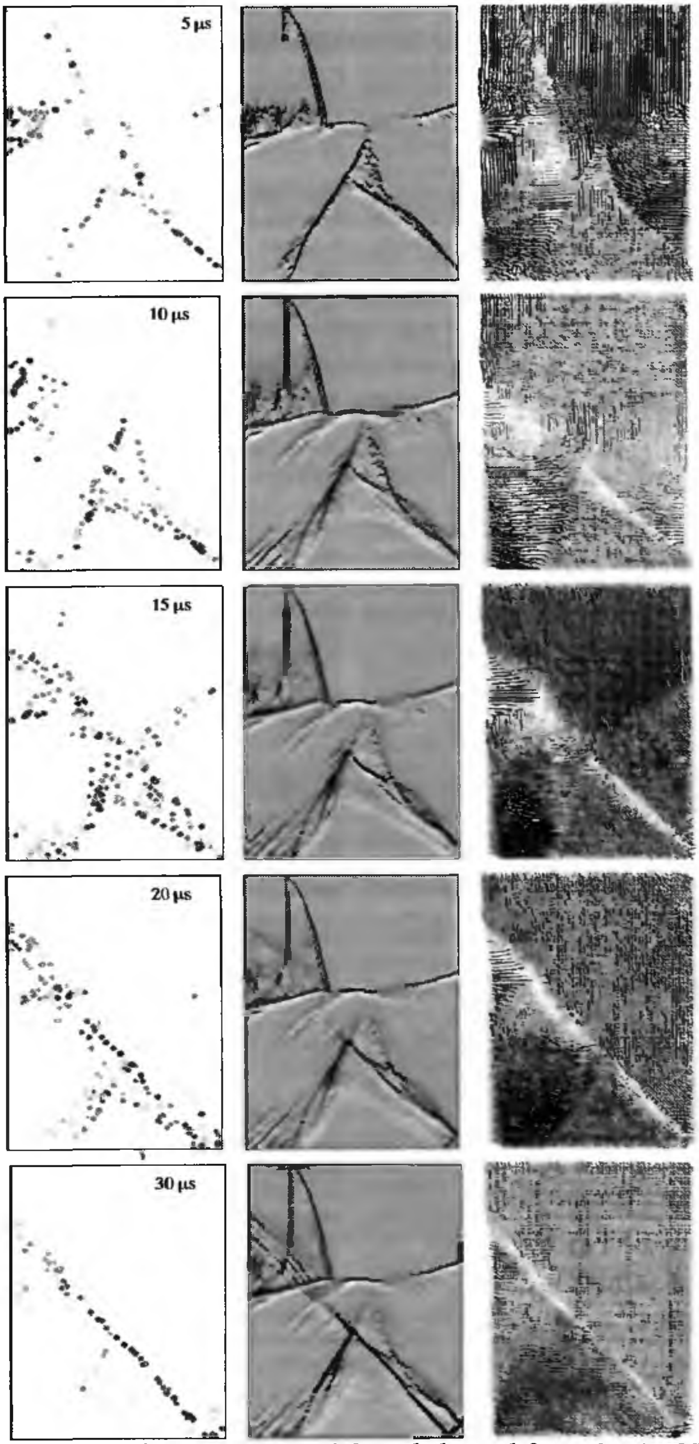

Figure 4. *Evolution of plastic strain rate (left) and plastic deformation (middle) patterns and velocity fields (right).*

to generate plastic shears and the front serves as a new source of intensive plastic deformation (see figs. 4a and -b). Referring to the last pictures in fig. 4, the old intergrain boundary blurs and practically disappears and the plastic shear front plays a role of interface between two fragments newly formed, which move each to other as separate parts. This process is similar to migration of the intergrain boundary.

4. Conclusion

This paper continues a number of works [1-5] devoted to modeling of elastoplastic behavior, taking into account generation of plastic shears by surface/interface sources and step-by-step propagation of plastic deformation. The advantages of the model we have made are relative to simulation of both repeat generation of shears by sources and plasticity development in crystal with slip planes.
Calculations have been performed for a model material, so that a quantitative comparison with experimental data is impossible to be done. It should be noted, however, that computational results have qualitatively described some phenomena experimentally observed. They are formation of mesocsale shear bands [8, 10], serrations in the stress-strain curve [11, 12], and evolution of intergrain boundaries [8-10].

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References

[1] Makarov, P., and Romanova, V., (2000), *Theor. and Appl. Fract. Mech.*, 33, pp.1-7.

[2] Romanova, V., Makarov, P., and Balokhonov, R., (2000) In: Proc. of the Third International Conference for Mesomechanics "MESOMECHANICS' 2000" (Xi'an, China), pp. 421-430, Tshinghua University Press, V.1.

[3] Romanova, V., (2000), *Physical Mesomechanics*, **3**, No.3, pp.71-76.

[4] Romanova, V., and Balokhonov, R., (2001), *Physical mesomechanics*, **4**, No.2, pp. 21-27.

[5] Makarov, P., Romanova, V., and Balokhonov, R., (2001), *Physical mesomechanics*, **4**, No. 5, (2001) pp.29-39.

[6] Wilkins, M., (1964), *Calculation of elastic-plastic flow. Methods in Computational Physics*, pp. 211, Academic Press, New York.

[7] Von Neumann, J., (1966), *Theory of self-reproducing automata*, Urbana, University of Illinois Press.

[8] *Physical mesomechanics of heterogeneous media and computer-aided design of materials*, (1998), Panin, V.E. (Ed), Cambridge International Science Publishing, Cambridge.

[9] Dudarev, E.F., (1998), *Microplastic deformation and yield point of polycrystals*, Tomsk University Press, Tomsk.

[10] Malis, T., Lloyd, D.J., Tangri, K., (1972), *Physica status solidi (a)*, **11**, No.1, pp.275–286.

[11] Panin, V.E., (1998), *Physical mesomechanics*, **1**, No.1.

[12] A. Ziegenbein, J., Plessing, J., Neuhaeuser, H., (1998), *Physical Mesomechanics*, **2**, No.1, pp.5–18.

[13] Toyooka, S., Widiastuti, R., Zhang, Q., and Kato, H., (2001), Jpn. Appl. Phys., 40 p.873.