Mesomechanics 2000

Volume I

Editor

G. C. Sih

Tsinghua University Press

MESOMECHANICS 2000

Role of Mechanics for Development of Science and Technology

Volume I

Role of Mechanics for Development of Science and Technology

Proceedings of an International Conference of Role of Mechanics for Development of Science and Technology, held at Xi'an Jiaotong University, Xi'an, China, June 13-16, 2000

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Volume I

Tsinghua University Press
Beijing, China

MESOMECHANICS 2000

Proceedings of the Third International Conference for Mesomechanics

Xi'an, P.R. China

Editor: G.C. Sih

Tsinghua University Press

Beijing 100084, P.R. China

Tsinghua

ISBN 7-302-00979-1/0 - 231 Set of 2 Volumes

Character of localized deformation and fracture of solids at mesolevel

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Abstract

Recent experiments have shown that shear band formation and rotation of structural elements at the mesolevel are fundamental to the development of plastic deformation and fracture of solids. Attention should be focused on a mesovolume of deformed material because the local stress and strain differ from those averaged at the macroscale. The discrete nature of the microshears and restricted deformation of the mesofragments should be accounted for. Rotation of the different mesofragments being parts of a grain, grains, grain conglomerates, etc., plays an important role in plasticity. Moreover, knowledge of the local parameters is needed for developing plasticity theories and fracture criteria. Models have been proposed within the framework of the physical mesomechanics. They take into account structural elements of different scales for simulating shear band nucleation and propagation in addition to mesofragment rotations. Calculations have been made for different mesovolumes under dynamic loading. In this work, a new criterion of plasticity is considered at the mesolevel. It accounts for the nucleation of plastic shears at the surfaces and interaction of structural elements. The numerical technique combines both the continuum mechanics approach and discrete cellular automata method.

1. Introduction

Traditional simulation of deformation and fracture of solids is made by application of continuum mechanics and averaged macroparameters. Knowledge of averaged data, however, is not sufficient for developing a predictive theory of deformed solids. Internal micro- and meso-structure evolution should also be considered as they affect the mechanical properties of materials. The invokement of continuum dislocation theory has had considerable success for describing the crystal deformation but it has not been able to describe macroscopic behavior of solids. Plastic deformation of materials appears to be localized in shear bands of different sizes involving the shear and rotation of the crystal lattice. Structural element interfaces such as grain and phase boundaries [1-3] contribute to the nucleation and propagation of plastic shears. The effect of load history involves a hierarchy of organized system of structural elements of different scales [4–6] with the capability of self-organization. Formation of shear bands of different degree is a fundamental character of all plastically deformed solids. The main factors involve stress concentrators at the mesolevel; interfaces of structural elements of different scales; shape changes of deformed structural elements; and localization of plastic deformation. They suggest that local values of the elastic-plastic flow parameters at the mesolevel differ widely from the averaged macrodata. Hence, a knowledge of the former could yield additional information for developing predictive theory of plasticity and fracture of solids. To reiterate, mesoscale investigation is important for its key role in continuum mechanics [4–6].

The concept of mesovolume is fundamental to this investigation where fluctuations of the local parameters can be taken into account. Mesovolume introduces the following features of the deformed continuum:

- slipping systems of the individual crystal and their activation under loading;
- nucleation and development of plastic shear bands; and
- initiation and propagation of internal non-compensating rotation of the structural elements.

Slip systems of individual crystals have been taken into consideration in a 2D formulation [5, 6] while this work discusses the third feature mentioned above.

Mesofragment rotation, magnitude of disorientation angles and components of the torsion-bending tensor measurements for plastically deformed polycrystals have been made in [7]. These results show that rotation of structural elements 10 μm or more in size occur in localized strain zone. The magnitude of rotation varies from a few degree to an order of magnitude larger. Torsion-bending tensor components are completely defined by extra dislocation density of similar sign $\rho_{\pm}$ as

$$\rho_{\pm} = \rho_{+} - \rho_{-} \approx \kappa_{ij} / |\mathbf{b}| \tag{1}$$

where $\mathbf{b}$ is the Burgers vector for dislocation and κ_{ij} are the torsion-bending tensor components. Experimental data show that $\kappa \approx 15$ deg/μm and $\Delta h \approx 0.15$ to 0.20 μm. Here, Δh is the characteristic size of the dislocation charge zone or the foil thickness with $\rho_{\pm} = 10^{11}$ cm^{-2}. These data can be used for analytical simulation of rotation and shear band formation at the mesolevel.

2. Simulation of plastic shear band nucleation and development

Conventional plastic flow treatment uses force to describe the onset of plasticity from a state of elasticity. The description is phenomenological using macroscopic material parameters. A quantity such as the yield point is used. The von Mises or Tresca condition has been commonly used.

Such an approach is incorrect for simulating plastic deformation at the mesolevel, where the stress-strain state may be non-uniform and the plastic deformation is highly localized [5, 6]. According to physical mesomechanics [4–6], plastic flow involves an evolution of shear stability loss at the micro-, meso- and macro-scale levels.

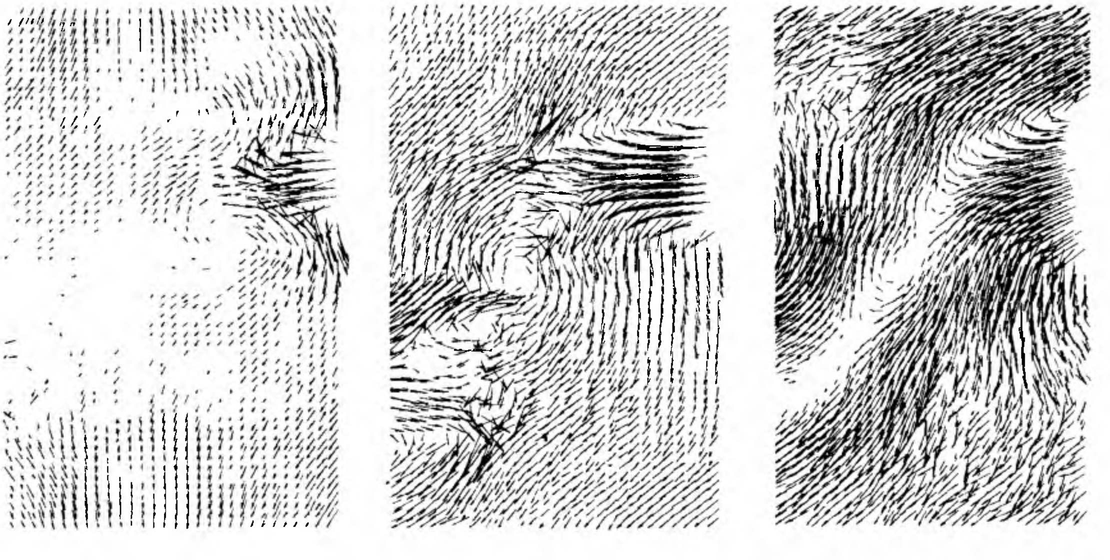
At the microscale level, the shear stability loss occurs in the localized zone of the crystal lattice involving the initiation and motion of dislocations. At the mesolevel, the shear stability loss is caused by the formation of mesobands in regions of localized deformation.

The initiation and subsequent growth of the shear bands lead to stress relaxation of the mesovolumes. Energy is required to generate the flow of deformation in the presence of defects. New dislocations could nucleate owing to hetergeneity at interfaces such as phase and/or grain boundaries or on the surface [1–3].

For shear stability loss to occur inside the individual crystals, it is necessary for shear stress to reach the theoretical shear strength of the crystal. Barring from such a high load, internal volumes of crystals are deformed elastically while the fronts of plastic deformation cover the elastic region. A definite level of dislocation density at the front is necessary for shear bands to propagate inward of the crystal. This corresponds to certain threshold value of deformation.

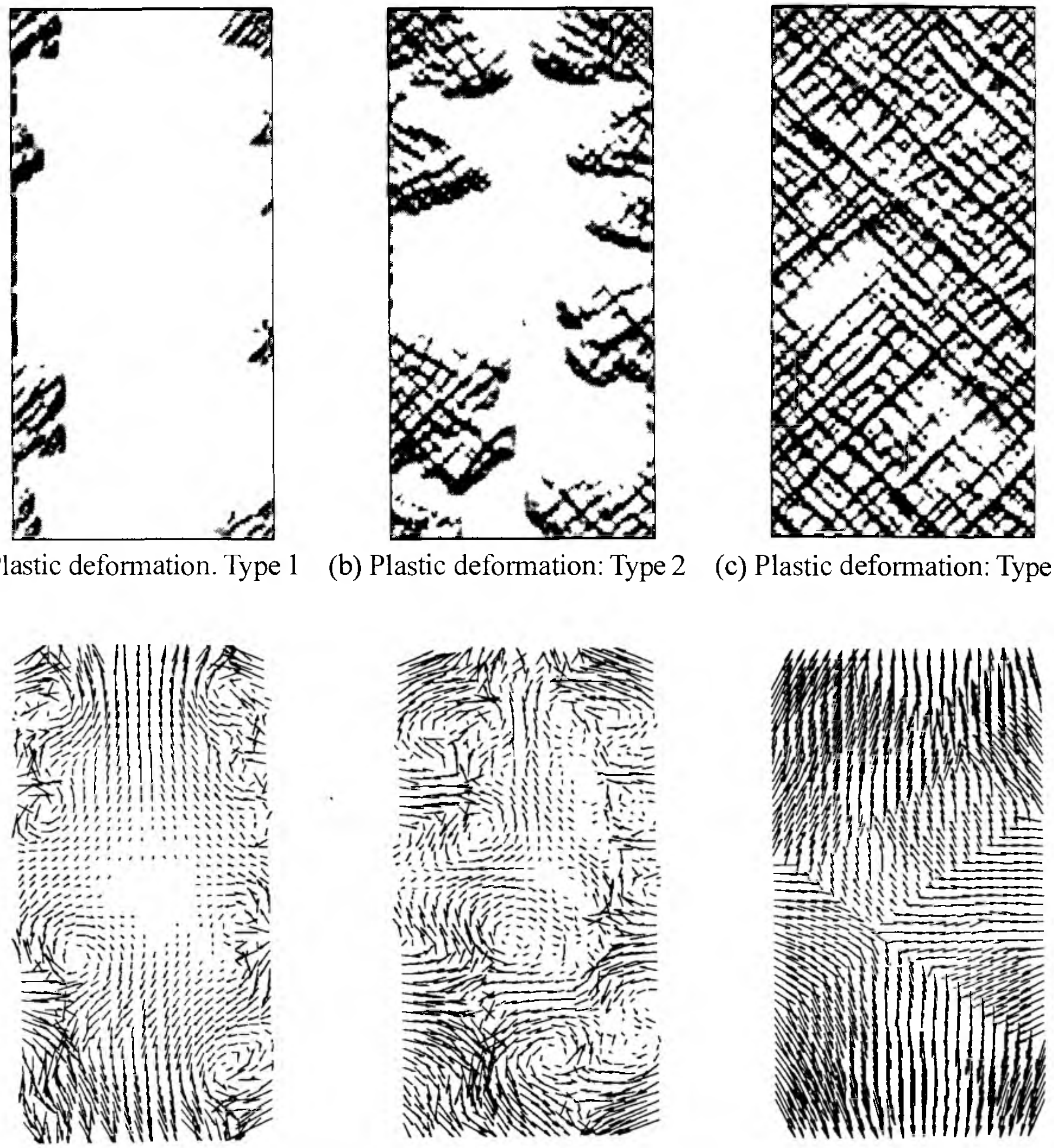
Conservation laws, elastic and plastic [6] constitutive equations are needed to perform numerical calculations and to develop a criterion of plasticity. In order to account for the physical process of shear band generation and development at the mesolevel, cell of computational grid referred to as a cellular automaton is introduced. The procedure can be stated as follows:

- The plastic shears can nucleate initially only at the surface of crystals or at different interfaces such as internal grain, phase boundary, boundary between inclusion and base material, etc.
- In order for the cellular automata to turn from an elastic to a plastic state, it is assumed that the effective stress σ_{eff} should reach a critical value σ^*. This value could be different for different structural elements such as surface, grain boundary, internal region of a grain, etc. Such a condition, however, is not sufficient.



(a) Time t_1 (b) Time t_2 (c) Time t_3

Fig. 1 Calculated velocity field of material in elastic-plastic state under tension [8]



(a) Plastic deformation. Type 1 (b) Plastic deformation: Type 2 (c) Plastic deformation: Type 3

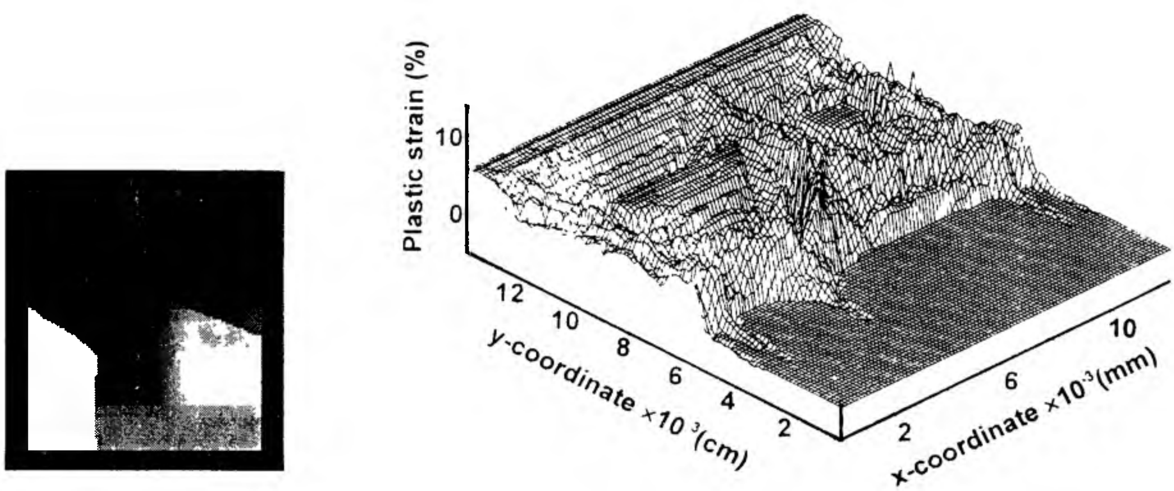
(d) Velocity field: Type 1 (e) Velocity field: Type 2 (f) Velocity field: Type 3

Fig. 2 Calculated strain and velocity data for different randomly distributed shear strength [8]

- The plastic flow can initiate in any internal cell, if the first condition is met. That is at least the plastic strain ε_{eff}^{p} in one of nearest cells has to reach the threshold value ε_{*}^{p}. The computational cell also becomes plastic if σ_{eff} has reached the value comparable with the theoretical shear strength σ_{cr}^{*}. In the latter case, the cell turns to a plastic state independent of the states (elastic or plastic) of the neighboring cells.

- If the above conditions are not fulfilled, the body continues to deform elastically. If cell becomes plastic, the stress would relax according to the prescribed constitutive relation..

Calculated results in [8] are shown in Figs. 1 and 2. Two conjugate mesoshear bands are seen to move from the specimen surface under tension. Fig. 2 shows the plastic deformation pattern and velocity fields for the case when the shear strength parameters have been randomly distributed throughout the specimen. Velocity field at the latter stages shows that the specimen has been separated into blocks that move in different directions. Calculated in [9] are results for a specimen consisting of several grains, shocked by a 3.7 GPa load. They are shown in Fig. 3(a). The distribution of plastic deformation after the shock wave front is shown in Fig. 3(b).



(a) Initial structure (b) Plastic strain distribution

Fig. 3 Polycrystalline specimen under 3.7 GPa shock wave load [9]

3. Simulation of independent rotation of mesofragments

Considered in [6] were simulation of shears in the base slip plane of polycrystalline grains. This work considers independent rotation of mesofragments. It is accounted by the asymmetric components of stress given as a function of the accumulated plastic deformation [6]. Suppose that the velocity field determines not only the displacements but the rotation of mesofragments as well. Asymmetric components of the stress tensor [6] is a function of plastic deformation accumulated or of plastic deformation gradient. Let the stress rate be defined as

$$\dot{\sigma}_{ji} = 2\mu\dot{\gamma}_{(ji)} + 2\alpha\dot{\gamma}_{\langle ji\rangle}, \quad \text{for } i \neq j \tag{2}$$

where the nonsymmetric strains γ_{ji} are introduced such that $\gamma_{(ji)}$ and $\gamma_{\langle ji\rangle}$ stand for the symmetric and asymmetric components, respectively. Knowing that

$$\dot{\gamma}_{ji} = \dot{\varepsilon}_{ji} - (\dot{\omega}_k - \dot{\Omega}_k)e_{kji} \tag{3}$$

with $\dot{\varepsilon}_{ji}$ being the standard symmetric strain rate and e_{kji} the Levi–Chevita tensor. The asymmetric part of strain can be written as

$$\dot{\gamma}_{\langle ji \rangle} = -(\dot{\omega}_k - \dot{\Omega}_k)e_{kji} \tag{4}$$

The antisymmetric stress components are given by

$$\dot{\sigma}_{ji}^{A} = -2\alpha(\dot{\omega}_k - \dot{\Omega}_k)e_{kji} \tag{5}$$

Considering the plane strain case

$$\begin{aligned} \dot{\sigma}_{12} &= \dot{\sigma}_{xy} = 2\mu\dot{\varepsilon}_{12} - 2\alpha(\dot{\omega}_3 - \dot{\Omega}_3) \\ \dot{\sigma}_{21} &= \dot{\sigma}_{yx} = 2\mu\dot{\varepsilon}_{12} + 2\alpha(\dot{\omega}_3 - \dot{\Omega}_3) \end{aligned} \tag{6}$$

Here,

$$\dot{\Omega}_k = -\frac{1}{2}\frac{\partial \dot{u}_\alpha}{\partial x^\beta} e_{\alpha\beta k} \quad \text{or} \quad \dot{\mathbf{\Omega}} = \frac{1}{2}\operatorname{rot}\dot{\mathbf{u}} \tag{7}$$

Note that $\dot{\mathbf{u}}$ is the velocity vector and $\boldsymbol{\omega}$ is the independent rotation vector. Under these considerations, $\boldsymbol{\omega}$ is a function of accumulated plastic strain ε_{eff}^{p} or plastic deformation gradient. That is

$$\omega_k = A_k \varepsilon_{eff}^{p} \tag{8}$$

where

$$\varepsilon_{eff}^{p} = \sqrt{3/2\, \varepsilon_{ij}^{p} \varepsilon_{ij}^{p}} \tag{9}$$

for the first case, and

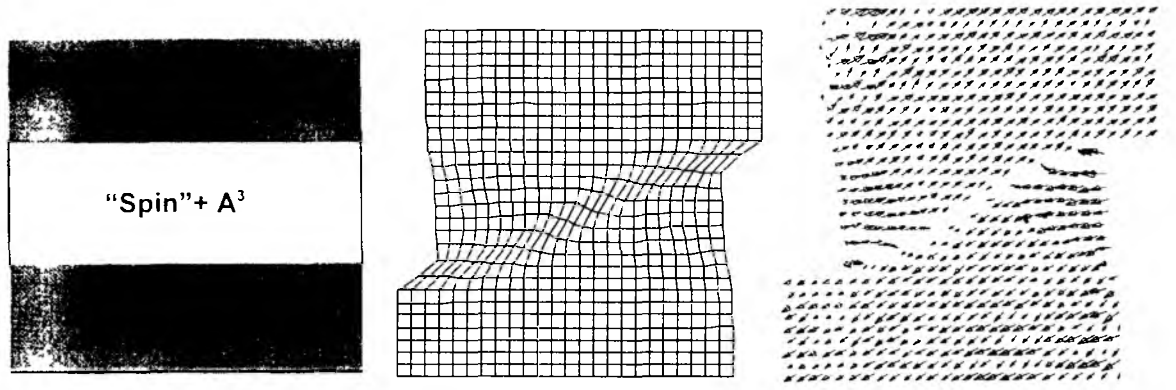
$$\omega_k = A'_k \left| \text{grad}\ \varepsilon_*^{p} \right| \tag{10}$$

or

$$\omega_k = -A'_\alpha \frac{1}{2} \frac{\partial \varepsilon_*^{p}}{\partial x^\beta} e_{\alpha\beta k} \tag{11}$$

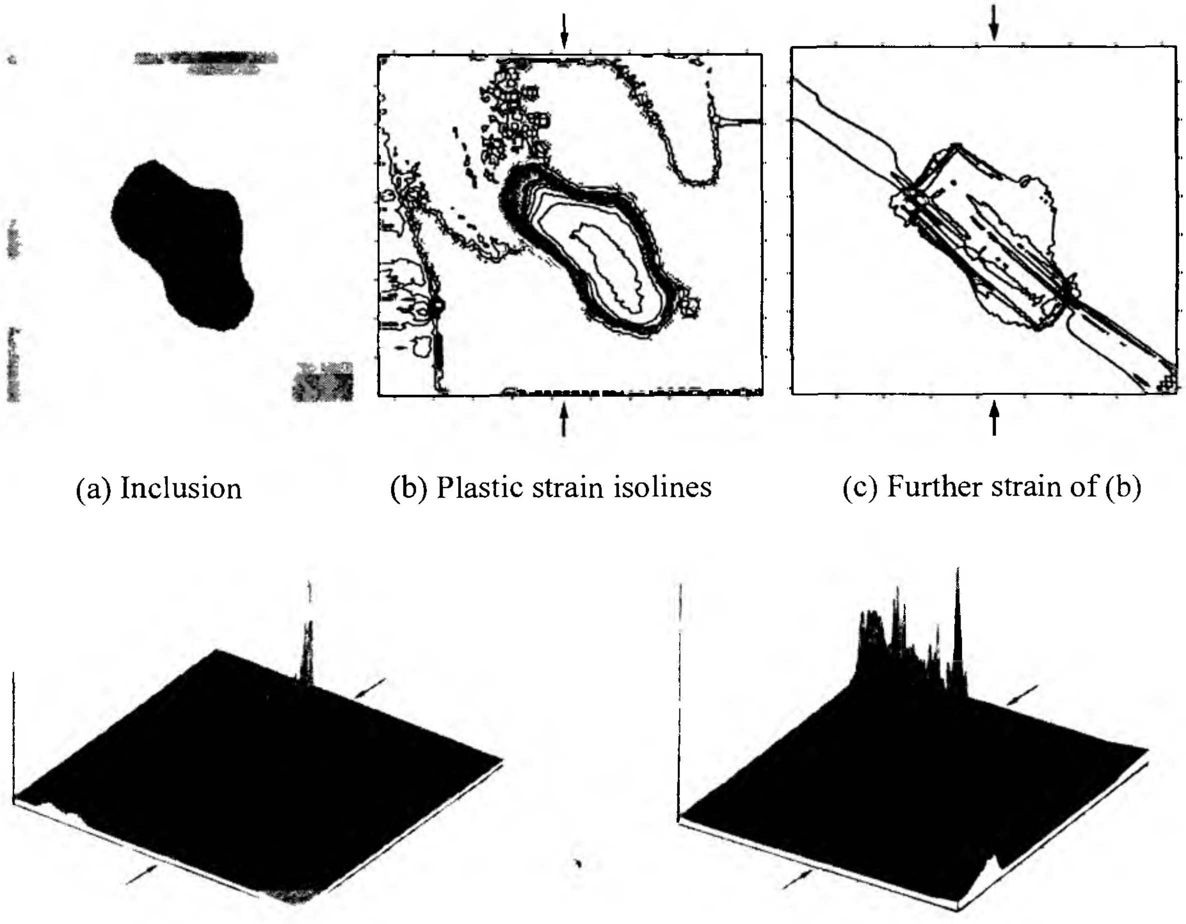
by analogy with Ω. For the two-dimensional case, $k = 3$ in eqs. (7) to (11).

The coefficient α in eqs. (2) and (6) determines the deviation of stress from the conventional elasticity theory where the stress tensor is symmetric. Indeed, test calculations show that the proposed model can simulate the behavior of crystals. Results of such calculations are shown in Figs. 4 to 6.



(a) Sandwich structure (b) Deformed grid (c) Velocity field

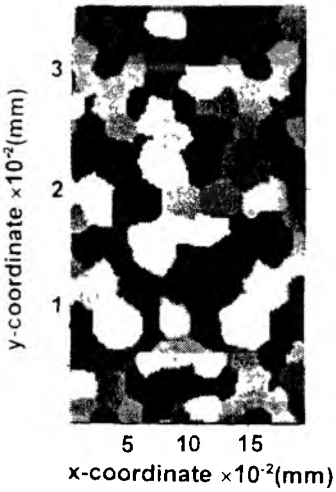
Fig. 4 Shear of sandwich structure and simulation results



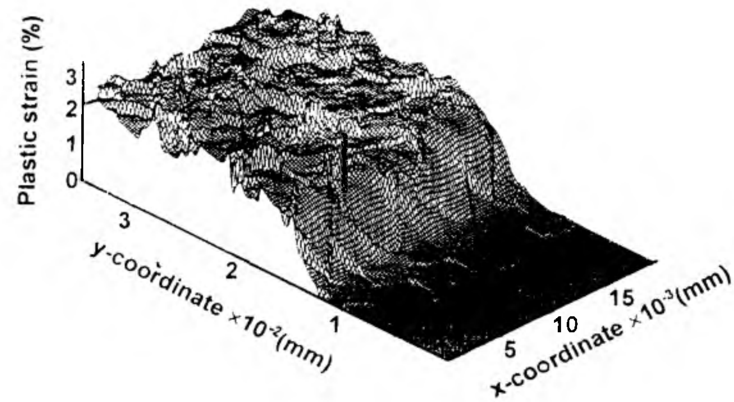
(a) Inclusion (b) Plastic strain isolines (c) Further strain of (b)

(d) Plastic strain distribution (e) Further strain of (d)

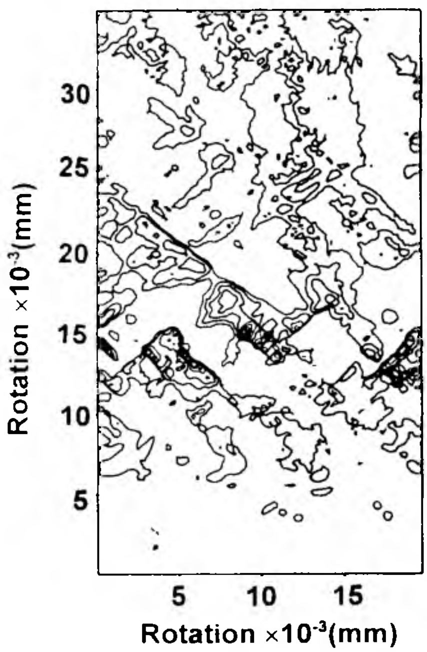
Fig. 5 Specimen under compression calculated by present model to exhibit rotation effect



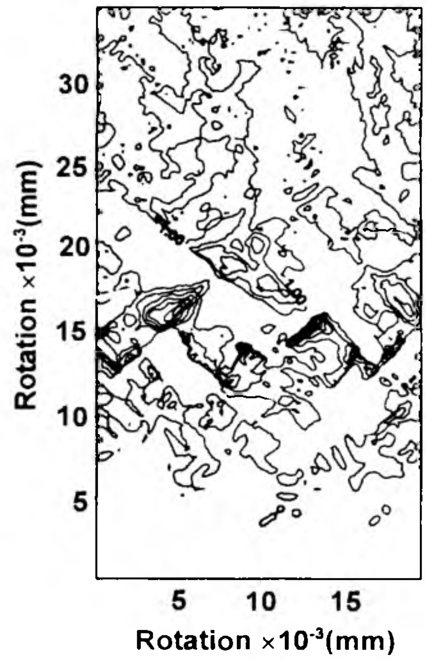
(a) Grain structure



(b) Plastic strain distribution



(c) Isolines of "+" rotation



(d) Isolines of "-" rotation

Fig. 6 Polycrystalline specimen subjected to 3.7 GPa shock load

Figs. 4(a) to 4(c) show the test calculation results for a "sandwich" structure whose interlayer has a "spin " with + A_3. The model used is defined by eqs. (8) and (10). The "plus" exerts a shear to the right while the element experience a clockwise rotation. The "minus " corresponds to a shear to the left and a counter-clockwise rotation of the element. Shear band formation data can be obtained from eqs. (8) and (11). Strain in the shear bands can be 150-200%, Fig. 4(b). Fig. 5(a) shows an inclusion embedded in an elastic-plastic matrix while Figs. 5(a) and 5(b) give the isolines of plastic strain. Near the inclusion boundaries the strain can be

100-200%, Fig. 5(b) while the total macrodeformation may only be a few percent. That is the local parameter at the mesolevel can be many times higher than those averaged at the macrolevel. Figs. 5(d) and 5(e) are elevation diagrams of plastic strain distribution. The results of a study for a polycrystal under shock wave loading with a magnitude of 3.7 GPa can be found in Figs. 6(a) to 6(d). The polycrystal grains structure in displayed in Fig. 6(a), Fig. 6(b) gives the plastic strain ε^{p}_{eff} distribution in the xy-plane. The isolines for "+" and "-" rotation are given, respectively, in Figs. 6(c) and 6(d).

Example data such as those in [7] for different materials can be used to determine the parameter in the computer simulation model presented.

4. Concluding remarks

Character of plastic deformation at the mesolevel requires the development of special models to describe the local plastic shear initiation, displacement and rotation of the material as a whole. These features necessitates a scheme for describing "shear + rotation " at the mesolevel. Moreover, the formation of conjugate shear bands and movements of the bulk structural elements should also be included. Special features of nonequilibrium behavior where fluctuations may be present also make the modelling more challenging, This may involve different physical and chemical process and phase transformations.

The criterion of plasticity at the mesolevel presented in this work takes into account the physical process of initiation and development of plastic shears. It makes possible the simulation of shear band propagation through the individual crystals from interfaces and surfaces. The combined use of continuous mechanics and discrete cellular automata has great promise for computer simulation of both the physical mechanisms of plastic deformation and fracture in addition to the physical and chemical process that may involve phase transformation.

Acknowledgement

The author wishes to thanks the co-workers for their assistance in the calculation. They include V.A. Romanova, D.V. Schmik and I.Yu. Smolin.

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