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POSSIBILITIES TO INCLUDE IN NUMERICAL SIMULATION STOCHASTIC AND DISCONTINUOUS PHENOMENA OCCURRING IN MATERIAL

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Abstract

Response of the CAFE (Cellular Automata in Finite Element) model for strain localization describing the stochastic character of deformation of the polycrystalline materials is presented in this work. Conventional models based on differential equations have some limitations in simulation of stochastic phenomena occurring in materials during processing. Contrary, CAFE approach offers a possibility of detailed investigation of those processes. Internal variables are defined for each particular CA cell, however particularly important for the model are variables correlated with stochastic behavior. They directly control transition rules, which describe micro shear bands and shear bands development. A detailed discussion of the advantages given by the developed multi scale CAFE model for strain localization phenomena, confronted to capabilities provided by the conventional FE approach, is a subject of this work. Results obtained from the CAFE model are validated by experimental observations, which show influence of discontinuities existing in the real material on the macroscopic response.

Key words: multi scale modeling, micro shear bands, finite element – cellular automata model

1. INTRODUCTION

Simulation of materials processing has to face new challenges, created by necessity of realistic description of various discontinuous and stochastic phenomena occurring in the deformed sample. Commonly used rheological models based on differential equations treat material as continuum and are unable to describe properly several important phenomena. Thus, there is ongoing search for alternative models, which can account for non-continuous structure of materials and for the fact, that various processes occur in different scales, from nano to mezo. Accounting for the stochastic character of some phenomena is an additional challenge. Multiscale approaches based on discrete models allow to overcome mentioned difficulties. One of the solutions is the coupled Cellular Automata (CA) – Finite Element (FE) multi scale model (Beynon et al., 2000; Shterenlikht, 2003).

Authors of the present work developed various multiscale models based on the CAFE methodology describing discontinuous processes occurring during the deformation i.e. strain localization (Madej et al., 2005; 2006a; 2006b). The problem of strain localization in materials during deformation is particularly important and have been investigated for over thirty years. A huge effort has been made to study experimentally and theoretically shear band propagation during various kinds of deformation. It has been observed that stress values in some deformation processes are significantly lower than obtained from common plastometric tests (Pietrzyk et al., 2004). Such effect is observed even in room temperature

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where thermal softening is not an issue. Experimental as well as inverse analysis based on ring compression RC, uniaxial compression UC and plane strain channel die test PSCc have revealed that the lowest values of stresses are in the PSCc test (Pietrzyk et al., 2004). It is commonly believed that development of micro shear and shear bands leading to strain localization is responsible for this decrease in stresses (figure 1). However, when propagation of micro shear and shear bands it is not precisely controlled, strain localization is becoming a precursor of material failure (figure 2). Potentials and threads related with strain localization development are reasons for intensive studies of this phenomena in many scientific laboratories.

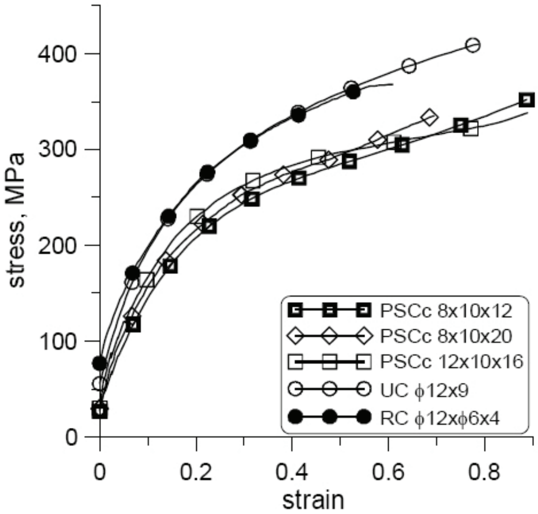

Fig. 1. *Stress vs. strain curves showing smaller values of stress in plane strain channel die compression in comparison with uniaxial compression (Pietrzyk et al., 2004).*

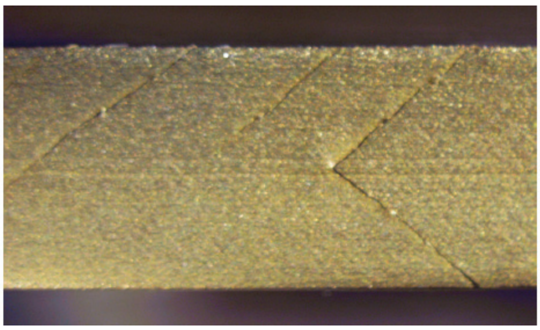

Fig. 2. *Crack initiation due to strain localization during flat rolling.*

As an outcome from these studies several forming processes, which benefit from the change of deformation path and shear band propagation, have already been designed and used in industry (Bochniak & Korbel, 2003). However, there is still lack of an efficient numerical model, which accounts for the influence of the shear bands, and which can properly describe material behavior during various FE simulations. Several attempts have been made to develop such a model (Pecherski, 1992; Wajda, 2004). Lack of flexibility and possibility of generalization is the main disadvantage of these models, which leads to difficulties when trying to simulate accurately real industrial processes.

An immense capabilities of the CAFE approach in comparison with the FE method limitations to model strain localization have already been reported in modeling of real material behavior (Madej et al., 2005a). The main objective of this work is detailed analysis of influence of the CAFE model stochastic part on material response in the conditions of plastic deformation. Beyond the multi scale nature of the proposed model, possibility of accounting for stochastic phenomena is the major advantage of the CAFE approach.

2. MULTI SCALE MODEL

The developed model is a real multi scale approach, which includes phenomena, taking place in different scales in the material, such as initiation and development of the micro shear and shear bands during various forming processes. Micro shear bands initiate in the micro scale, while shear bands occur in the mezo scale. For the conventional FE approaches modeling of the phenomena appearing simultaneously in different scales is difficult. Usually size of the FE elements is selected to be between scales of those two phenomena, what influences the accuracy and increases computation costs. In the CAFE approach it is not an issue, because two separate CA spaces are introduced to deal with those two phenomena. First CA space describes development of micro shear bands and the other describes development of shear bands. A schematic illustration of the multi scale nature of the CAFE model is presented in figure 3.

CA spaces have to be precisely defined, before attaching to each particular integration point. The same procedure is performed for both micro shear band space (MSB space) and shear band space (SB space). In the CAFE model both CA spaces are characterized by several state variables, describing each particular cell, as well as by a set of transition rules defined respectively for those spaces. These rules are based on the knowledge regarding the specific phenomenon (Bochniak & Korbel, 2003; Korbel, 1998; Cizek, 2002). The author of (Cizek, 2002) claims that micro shear bands develop through the formation of slip domains, which are discrete cells aligned along the band propagation direction. The misorientation angles between those cells and the surrounding matrix increase during the progress of deformation. They form narrow bands that, afterward, become thicker due to the formation of new cells. Beyond this, it is stated in (Korbel, 1998) that development of micro shear bands is due to employing a coarse slip system in the grain, and development of the shear band is connected with micro shear bands clustering in the material. The theory of (Korbel, 1998) describes the micro shear band and shear band phenomena as two processes, which take place in two different scales in the material at the same time. Micro shear bands are usually related with one particular grain or several adjacent grains while shear bands are crossing grains independently of their orientation.

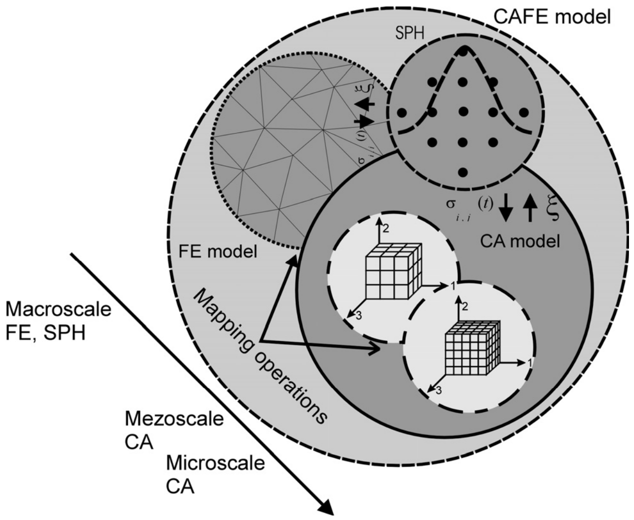

Fig. 3. *Complete multi scale CAFE model with the SPH interpolation part applied to solve problems with remeshing (Madej et al., 2005b).*

However, idea of crystallographic or non-crystallographic character of micro shear bands is the fundamental problem on which there is still no agreement. The opinion that SBs are non-crystallographic derives from macroscopic observations and general considerations of the stability of the C(112)[11$\bar{1}$] orientation at high strains, as initially proposed by (Morii et al., 1985). The second argument advocated by the authors quoted non-crystallographic character of SBs results from the observation that macroscopically observed shear occurs in a plane different than {111} plane in the matrix outside the band. In opposition, the concept regarding crystallographic nature of SBs assumes their formation as a result of local lattice re-orientations within narrow areas.

All those experimental observations are a source of knowledge which is used by the authors to create transition rules, which are created for MSB and SB spaces (Madej et al., 2006a; 2006b). Only part of the model, responsible for stochastic behavior related with micro shear bands development, is described in this paper. After creation of internal variables and transition rules the CA spaces are defined and attached to each particular integration point in the FE mesh. The following internal variables are introduced to the MSB space: *state* – representing the state of each cell, *old state* - representing the state of each cell in the previous time step, *rotation angle* – describing the cell rotation, *old rotation angle* – describing the cell rotation in the previous time step, *tau_h*, – critical values of stress necessary to initiate hard slip system in the material. Each MSB cell can be in two possible states: *nonactiveMSB* and *activeMSB*. The *activeMSB* state indicates that micro shear band was initiated and develops in this cell, while a *nonactiveMSB* state refers to the surrounding matrix. The remaining variables are more related to the micro shear band phenomena rather than to CA theory.

At the beginning of deformation process, critical values of variables describing stresses are generated for each MSB cell using the gauss distribution function (figure 4):

$$\tau_{hard} = \frac{1}{\sigma_{dev}\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma_{dev}^2}} \qquad (1)$$

where: x – expected value, σ_{dev} – standard deviation.

This process is responsible for initiation of the hard slip system in the MSB spaces, and is directly related with the initiation of micro shear band mechanism described in (Cizek, 2002). This approach is used instead of explicit inclusion of grain orientations in the area of the sample. That is one of the most important steps to reproduce real behavior of the polycrystalline material.

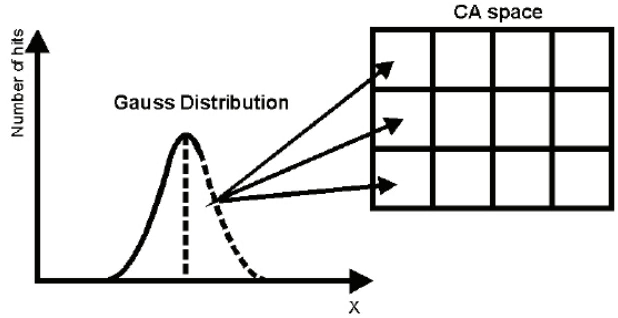

Fig. 4. *Illustration of the generation of internal variable tau_h.*

Transition rule, that provides change from the *nonactiveMSB* to *activeMSB* state, is described as:

$$Y_{m(MSB)}(t_{i+1}) = \begin{cases} activeMSB \Leftrightarrow A \\ Y_{m(MSB)}(t_i) \end{cases}$$

$$A = \left(\sigma_i > \tau_{hard}\right) \vee$$

$$\text{where: } \begin{pmatrix} Y^m_{l(MSB)} = activeMSB \wedge \\ \theta^{rot}_m - \theta^{rot}_l > \theta^{rot} \end{pmatrix} \qquad (2)$$

where: $Y_{m(MSB)}\left(t_{i+1}\right)$ – state of the m^{th} cell from the MSB space at the t_{i+1} time step, σ_i – equivalent stress value obtained from the FE program, τ_{hard} – critical value for initiation of the hard slip system, $Y^m_{l(MSB)}$ – state of the l^{th} neighbor of the m^{th} cell from the MSB space, θ^{rot} – rotation angle.

Each particular cell can change its state to *activeMSB* when an equivalent stress value obtained from FE code exceeds a critical value, which is necessary to initiate hard slip system in the material generated for each particular cell according to (1). This part of the transition rule have a nondeterministic character due to application of the Gauss distribution function.

However during creation of the second part of the transition rule a probabilistic change of one of the parameters have been introduced, as well. When a neighbor of a selected cell in the previous time step was *activeMSB* and the rotation angle between those two cells is above certain critical value, cell changes its state to *activeMSB*. One of the key parameters in this part is internal variable describing *rotation angle* θ^{rot}, directly related with the process shown in figure 5 (Cizek, 2002).

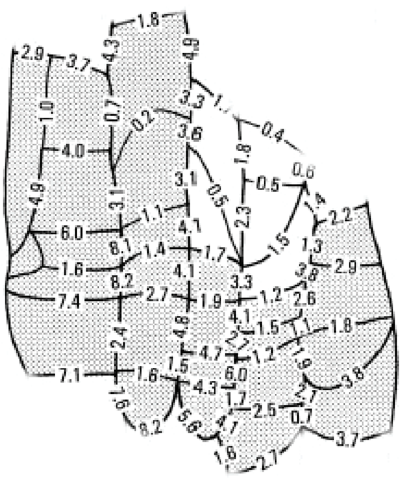

Fig. 5. *a) misorientations map with the domain misorientation values (Cizek, 2002).*

It is shown in figure 5 that misorientation angles of the cell boundaries reach values higher than 8°. Eventually they form narrow bands that afterward become thicker, due to the formation of the new cells. This process is connected with micro stress fields generation during the rotation of the previously formed cells, leading to initiation of micro shear band. This statement is directly related with the second part of the described transition rule, particularly with *rotation angle* internal variable. In each time step *rotation angle* for cells in the *activeMSB* state changes in a probabilistic manner.

Those two main parameters, *tau_h* and *rotation angle*, are responsible for changes in the cells interactions in the MSB space, as well as in interactions between MSB and SB spaces, what is crucial in the process of shear band development.

The main idea of the CA theory is to create a set of rules controlling changes between cells state to properly describe real processes. Due to that, all mentioned above work to replicate processes such as development of micro shear band and shear band propagation resulted in creation of the model capable of prediction material behavior in a stochastic and not only deterministic manner. That is one of the main advantages of the developed approach. Results describing this stochastic character of the CAFE model are presented in the next section.

3. RESULTS

Calculations using the CAFE model for strain localization were performed for the simple compression in the channel die test. Presentation of the stochastic character of the model is the main objective of these simulations. The channel die test is a kind of the plane strain compression test, in which material flow is constrained by an additional tool. Since the plane strain condition fosters initiation of shear bands, this test is commonly used to investigate strain localization (Anand & Spitzig, 1980). It is commonly expected that the strain distribution field in the channel die tests reflects the metallurgical cross. Such stress conditions favor development of the shear banding mode of deformation. Results obtained from 10 simulations performed for the same process parameters are presented in figure 6.

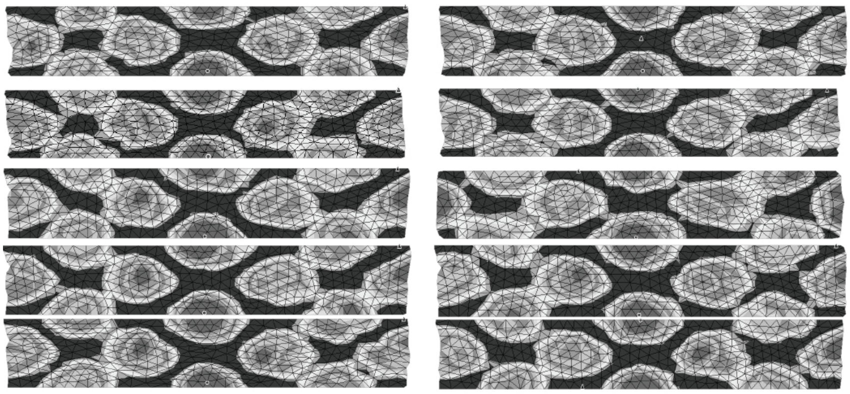

Fig. 6. *Cross section of 10 samples illustrating differences in final shape obtained for the same process conditions.*

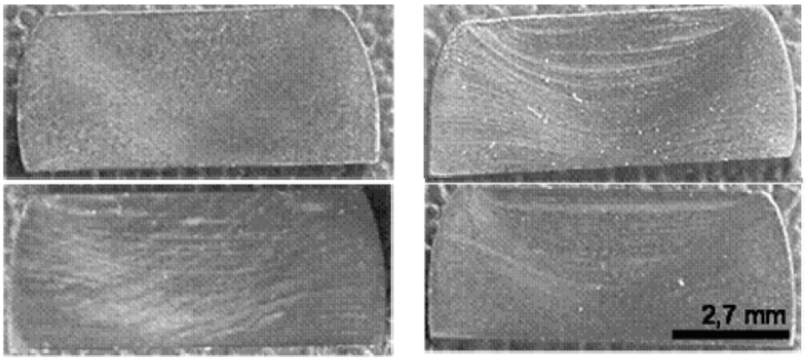

Fig. 7. *Shape of the polycrystalline copper samples after channel die test performed for the same process conditions.*

It is clearly seen in figure 6 that strain distribution field vary slightly between specific cases but global material response is the same. The non deterministic character of metal flow is well visible when shape of the sample is considered. Sample shape in each case is again slightly different, what reflects real material behaviour. In real experimental tests the same process never ends with exactly the same shape of the sample, what is shown in figure 7.

That behaviour is a natural outcome from the material polycrystalline character. But this behaviour cannot be modelled using the conventional and continuous approaches, where final results for the process performed with exactly the same parameters always gives the same response. As it s shown in the paper, the CAFE model does not have that limitation and all the obtained results are closer to real material behaviour.

4. CONCLUSIONS

Developed CAFE model is capable of including stochastic phenomena which occur during deformation at different scales in the material. This multi scale nature and non deterministic behavior are the major advantages of the developed approach. Those capabilities create possibilities of detailed investigation of problems occurring in real industrial processes. Since stochastic parameters have a significant influence on material behavior, it is crucial to identify the parameters, which have the largest influence on obtained results. Presented work is part of the general effort leading to proper validation and calibration of the proposed model. An analysis of model's sensitivity to changes of its parameters will be performed during further work.

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ANALIZA MOŻLIWOŚCI SYMULACJI NUMERYCZNEJ ZJAWISK O CHARAKTERZE STOCHASTYCZNYM I NIECIĄGŁYM ZACHODZĄCYCH W MATERIALE

Streszczenie

Stochastyczny charakter procesu lokalizacji odkształcenia analizowany w oparciu o model analizy wieloskalowej CAFE przedstawiony jest w niniejszej pracy. Konwencjonalne modele numeryczne bazujące na równaniach różniczkowych nie są w stanie opisać zjawisk o charakterze stochastycznym, z kolei model CAFE jest pozbawiony takiego ograniczenia. W pracy omówiono zmienne wewnętrzne zdefiniowane w przestrzeniach automatów komórkowych związane ze stochastyczną odpowiedzią modelu. Zdefiniowane zmienne wewnętrzne bezpośrednio wpływają na stworzone reguły przejścia opisujące propagacje mikro pasm i pasm ścinania. Zalety proponowanego rozwiązania są poddane dyskusji i porównane z wynikami przeprowadzonych badań doświadczalnych.

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