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# MULTI SCALE MODEL FOR PREDICTION OF MATERIAL BEHAVIOR DURING DEFORMATION PROCESSES

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**Summary.** *A multi scale Cellular Automata – Finite Element model for prediction of initiation and propagation of micro shear bands and shear bands in metallic materials subjected to plastic deformation was developed. The concept of the model is described in the paper and the transition rules for the cellular automata are defined. In defining the rules, particular emphasis was put on accounting for the physical aspects of the phenomena, which take place in the material at micro and mezo scales. Selected examples of applications of the developed model to simulations of metal forming processes, which involve strain localization, are presented.*

## 1 INTRODUCTION

Recent scientific experiments have shown that prediction of an initiation and development of micro shear bands and shear bands is crucial for accuracy of modeling of plastic deformation in variety of metallic materials. Those phenomena have been experimentally and theoretically studied over recent years by several researchers [1,2]. Traditional way of modeling strain localization in the material during deformation processes is based on the Finite Element technique (FE), which is capable of modeling shear bands development. However, results of those simulations are still not satisfying. There is a lack of the rheological model, which predicts the micro-shear and shear band propagation in the sample under various complex deformation processes. The alternative solution for predicting phenomena, which take place during the deformation in different scales at the same time, is coupled Cellular Automata (CA) – Finite Element (FE) multi scale model. The CAFE approach was successfully used for modeling the microstructure evolution during hot rolling[3] as well as for modeling of the ductile-brittle fracture[4]. The objective of the present study is development of CAFE approach for modeling strain localization, which will become an efficient tool for modeling material behavior under various loading conditions.

## 2 MULTI SCALE APPROACH

In the coupled CA and FE approach, a discrete cellular automata are introduced and attached to each particular FE integration point. CA technique gives a possibility of modeling of material behavior in the nano, micro or mezo scales. That was the reason why cellular automata were used for creation of the multi scale analysis CAFE model by combining the advantages of the CA with the FE method.

Such phenomena as micro-shear and shear band development take place in two different scales in the material: micro-shear bands (MSB) take place in the micro-scale, while shear bands (SB) occur in the mezo-scale. According to those differences, two CA spaces describing the material behavior in those two scales are introduced and are attached to the finite elements, which handle the calculation of material behavior in the macroscopic scale.

In the CAFE approach each cell in the CA spaces is described by several state variables and precisely declared transition rules defined according to the physical basis of the phenomena, which are taken into consideration during deformation process. For the MSB space, internal variables describing state, rotation angle and value necessary to initiate a hard slip system in the material were introduced. A particular MSB cell can be in the two possible states – *nonactiveMSB* and *activeMSB*. A state *activeMSB* indicates that micro-shear band development takes place in the cell, while a *nonactiveMSB* refers to the surrounding matrix. In the SB space only two state variables are defined: state variable and micro-shear band fracture $\alpha$ (MSB fracture) variable. Parameter $\alpha$ is calculated according to the number of cells in the *activeMSB* state and has values between $\langle 0{,}1 \rangle$. That leads to three possible states of the SB cell: *nonactiveSB*, *activeSB*, *activeMSB*. State *activeSB* refers to a cell, in which a shear band appears during calculation. *NonactiveSB* is used to describe the surrounding matrix. State *activeMSB* refers to a SB cell, in which micro-shear bands in the underlying MSB space have developed.

Transition rules controlling changes between states in the MSB and SB spaces are defined, based on the experimental knowledge[1,2]. Transition rules, which provide a change from *nonactiveMSB* to *activeMSB* state, are described by:

$$\Upsilon_{m(MSB)}(t_{i+1}) = \begin{cases} activeMSB \Leftrightarrow A \\ \Upsilon_{m(MSB)}(t_i) \end{cases} \quad \text{where } A = \left(\sigma > \tau^*_{\max}\right) \vee \left( \begin{array}{l} \Upsilon^m_{l(MSB)} = activeMSB \wedge \\ \theta^{rot}_m - \theta^{rot}_l > \theta \end{array} \right) \qquad (1)$$

where: $\Upsilon_{m(MSB)}(t_{i+1})$ – state of the $m^{\text{th}}$ cell from the MSB space at the $t_{i+1}$ time step, $\sigma$ - stress value obtained form the FE program, $\tau^*_{\max}$ - critical value for initiation of the hard slip system, $\Upsilon^m_{l(MSB)}$ - state of the $l^{\text{th}}$ neighbor of the $m^{\text{th}}$ cell from the MSB space, $\theta$ - rotation angle.

In the SB space, a cell state *activeMSB* is used for creation of the link between MSB and SB spaces. It is stated in[1] that shear banding phenomena develop based on the previously formed micro-shear bands. Information about the propagation of micro-shear and shear bands is exchanged between the CA spaces during each time step, according to the defined mapping functions. Change between the states is due to the following transition rules:

$$\Upsilon_{m(SB)}(t_{i+1}) = \begin{cases} activeSB \Leftrightarrow A \\ \Upsilon_{m(SB)}(t_i) \end{cases} \quad \text{where} \begin{array}{l} A = \left(\Upsilon_{m(SB)}(t_i) = activeMSB \wedge \alpha_m(t_i) > \alpha_{cr}\right) \\ \vee \left(\Upsilon^m_{l(SB)}(t_i) = activeSB\right) \\ \vee \left(\Upsilon^m_{l(SB)}(t_i) = activeMSB \wedge \alpha_m(t_i) > \alpha_{cr}\right) \end{array} \tag{2}$$

where: $\Upsilon_{m(SB)}(t_{i+1})$– state of the $m^{\text{th}}$ cell from the SB space at the $t_{i+1}$ time step, $\Upsilon^m_{l(SB)}$ - state of the $l^{\text{th}}$ neighbor of the $m^{\text{th}}$ cell from the MSB space.

In each time increment information about stress tensor is sent from the finite element solver to the MSB space, where development of micro-shear bands is calculated according to equation (2). After exchange of information between CA spaces, development of the shear band is predicted based on equation (1). A value of the equivalent stress $\sigma_p^{CA}$ is calculated as an outcome from CA calculations and is used to obtain correction coefficient $\xi$ :

$$\xi = \frac{\sigma_p^{CA}}{\sigma_p^{FE}} \tag{3}$$

This coefficient is used in the FE model to modify the flow stress values in each particular gauss point during next step of calculations.

## 3 RESULTS

The change of the state of a selected cell depends on the state of this cell and its neighbors in the previous time step. According to this essential definition of the CA method, a number of CA spaces in the CAFE approach should remain constant during the calculations. It creates problems when a complicated schemes of deformation or sample shapes are introduced and a remeshing is applied. It leads to a change in the number of the nodes as well as in number of the integration points and, apparently, to a problem with attaching of the CA spaces to the FE nodes. Lack of information from the micro-scale in some regions of the FE mesh may follow and, eventually, erroneous results may be obtained. Thus, in this work an alternative set of points is introduced in the sample to overcome this problem. A number of so called CA points remain constant during the deformation process and a number of underlying CA spaces attached to each CA point remains constant, as well. This approach enables remeshing and change of the number of the nodes. In each time step an exchange of information between FE points and CA points is performed using the Smoothed Particle Hydrodynamics method[5,6] (SPH). That is a two step process. First the approximation of the displacement filed is performed. After updating of the CA point position the approximation of the stress filed is performed.

Calculations using the CAFE model for strain localization combined with the SPH approximation method were performed for the simple compression in the channel die test. Results of simulations using the conventional FE method and CAFE approach are compared in figure 1. The CAFE model is based on the commercial FORGE 2 program and on the CA code developed by the authors.

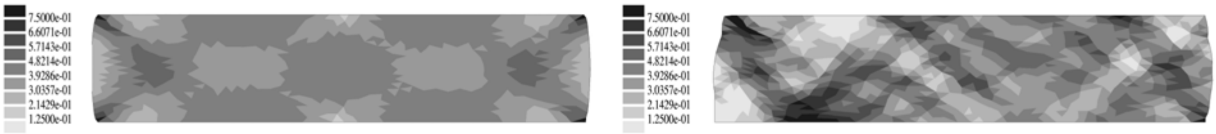

Figure 1. Strain distribution during the channel die tests, calculated by the conventional FE model (left) and by the developed CAFE model (right).

It is clearly seen in Figure 1 that a strain localization in the bands appears when the CAFE approach is applied. This is due to the development of the micro-shear and shear bands in the micro and mezzo-scale, respectively, during the deformation process. Similar results obtained with the CAFE model without approximation module are presented in[7].

## 4 CONCLUSIONS

The CAFE approach is a multiscale model, which performs calculations in different scales in the material and accounts for stochastic phenomena, which take place in the materials during deformation. The primary results obtained from the strain localization CAFE model describe reasonably well a real material behavior and prove predictive capabilities of this approach. Application of the SPH method in the CAFE model allows to overcome the remeshing problem. Combination of the SPH and CAFE approach creates a multi scale model, which is easily applicable to different deformation processes.

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