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MODELING OF THE INITIATION AND PROPAGATION OF THE SHEAR BAND USING THE COUPLED CAFE MODEL

PRZEWIDYWANIE POWSTAWANIA I PROPAGACJI PASM ŚCINANIA W STALACH Z WYKORZYSTANIEM HYBRYDOWEGO MODELU CAFE

A study of the possibilities given by the multi scale CAFE method for the parallel modeling of the microshear and shear band propagation in steels during deformation is presented in this work. The developed model is based on the idea of multi scale CAFE approach developed at Sheffield University in England, and used for the Charpy test modeling. Modeling of the microshear bands development in microscale, shear bands development in mezoscale and material response based on those processes in macroscopic scale is possible using this multi scale computational technique. The models composing space of cells, definition of neighborhood and definition of transition rules for two problems, crack initiation in the deformed materials and development of micro shear bands, is described in the paper. Both models are implemented into the finite element code. The results of simulations of Charpy tests and compression in channel dies are presented.

Keywords: multi scale modeling, cellular automata, shear bands

Niniejsza praca stanowi wstęp do badań nad możliwościami zastosowania metody CAFE do modelowania zjawiska powstawania i propagacji pasm ścinania w odkształcanym materiale. Opracowywany model bazuje na metodologii wieloskalowej analizy CAFE opracowanej w przeciągu ostatnich czterech lat na Uniwersytecie Sheffield w Wielkiej Brytanii i z powodzeniem zastosowanej do modelowania testu Charpy'iego. Poprzez zastosowanie tej metody możliwe jest jednoczesne modelowanie zjawisk zachodzących w mikroskali — powstawanie mikropasm ścinania, mezoskali – rozwój makropasm ścinania, oraz makroskali — odpowiedź materiału na powyższe zjawiska. W pracy przedstawiono opis modelu obejmujący przestrzenie komórek oraz definicje sąsiedztwa i reguł przejścia dla dwóch zagadnień, propagacji pęknięć w materiałach odkształcanych oraz rozwoju mikropasm ścinania. Obydwa modele zostały połączone z programem z metody elementów skończonych. W pracy przedstawiono wyniki symulacji próby Charpy'ego oraz plastometrycznej próby kanalikowej.

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1. Introduction

Recent scientific experiments have shown that initiation and development of micro shear bands and shear bands are crucial for the development of plastic deformation in a variety of metallic materials [1, 2]. The traditional way of modeling a material's behavior during the deformation process is to use the Finite Element technique (FE), which is capable of predicting the occurrence of material instability such as fracture, strain localization, and many other instabilities. This technique is commonly used in scientific laboratories.

However, when using traditional FE modeling, it is very difficult to predict phenomena, which take place in different scales in the material during the deformation process. The search for an alternative computational method has been carried out for several years. One of the solutions may be the coupled Cellular Automata (CA) — Finite Element (FE) multi scale model. The CAFE approach has already been successfully used for modeling the microstructure deformation during hot rolling [3] as well as for modeling the ductile-brittle fracture [4] during the Charpy test. In the CAFE approach material behavior can be completely separated from the structural response because calculations are coupled between the cellular automata technique and the finite element method.

The objective of the present work is adaptation of the idea, which is used in [4] for modeling cracks propagation, to predict initiation and development of micro shear bands. The model of [4] is described briefly and selected results of simulations are presented. Following this, a new model for micro shear bands is proposed.

2. CA basis

The cellular automata approach was originally developed in early 1960s of the last century by Janos Von Neumann [5] for simulating the behavior of discrete, complex systems. This technique is becoming more popular with the ever increasing computational power of today's computers. Nowadays the CA method is already used in different scientific areas from biology and chemistry to solid phase physics and electronics. During the last few years CA has also been applied in several attempts to model material behavior during plastic deformation. Several works, which include modeling of static and dynamic recrystallization behavior, can be found in scientific literature [6, 7].

The main idea of the cellular automaton technique is to divide a specific part of the material into one-, two-, or three-dimensional lattices of finite cells. Each cell in this space is called a "cellular automaton," while the lattice of the cells is known as "cellular automata space." Each cell in this CA space is surrounded by neighbors (Figure 1), which affect one another. Neighborhoods can be specified in one, two, and three dimensional spaces. Several examples of neighborhoods can be found in different applications of the CA method. The most popular examples are the von Neumann and

the Moore neighborhoods where in the 2D case each cell is surrounded by four and eight neighboring cells, respectively. But there are also examples of alternative shapes of CA neighborhoods such as hexagonal neighborhoods [8].

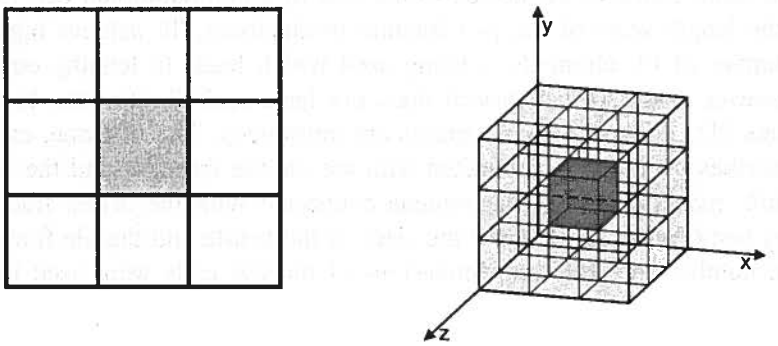

Fig. 1. Moore neighborhood in 2D and 3D space

The interactions of the cells within the CA space are on the bases of the knowledge defined while studying on a particular phenomenon. In every time step, the state of each cell in the lattice is determined by the previous states of its neighbors and itself, by a set of precisely defined transition rules f:

$$\gamma_i^{t+1} = f(\gamma_j^t) \quad \text{where} \quad j \in N(i) \tag{1}$$

Where: $N(i)$ — surrounding of the i^{th} cell, γ_i — state of the i^{th} cell.
Since the transition rules control the cells' behavior during calculations (i.e., during the deformation process), the proper definition of these rules is crucial in the process of designing a CA model.
The CA method is commonly used for modeling materials' behavior in the nano, micro, or mezo scale. When the advantages of this method are combined with the advantages of the macro scale analysis — FE method, a complete multi scale analysis model such as the CAFE model can be created.

3. CAFE models

The main objective of this work was to develop of the 3D multi scale CAFE model for the prediction of micro shear bands and shear bands development during the deformation process. The inspiration was the CAFE model created by Shterenlikht at The University of Sheffield in England [4], which described propagation of the brittle and ductile fracture in material during the Charpy test. Short description of this approach is described in the following part of this paper.

Brittle and ductile fractures are the two phenomena, which take place in the two different scales in the material during deformation. The length scale of the brittle

fracture is 0.005-0.05 mm, and the scale for the ductile fracture is 0.1-0.5 mm. The small scales of these phenomena are the reasons why modeling is very difficult. In conventional FEM modeling, the brittle and ductile fractures are modeled using the size of the finite elements connected to the size of a computational cell [9] which is between the length scale of the two fracture mechanisms. To achieve high accuracy, a large number of FE elements is being used which leads to lengthy computational times. However, the CAFE approach does not have such limitations. In this model two separate 3D cellular automata spaces are introduced. The first one, called *ductile space*, describes phenomena connected with the ductile fracture, and the second one, called *brittle space*, describes phenomena connected with the brittle fracture during the Charpy test (Figure 2). Because the sizes of the brittle and ductile fractures differ, a different number and different dimensions of the CA cells were used in those CA spaces.

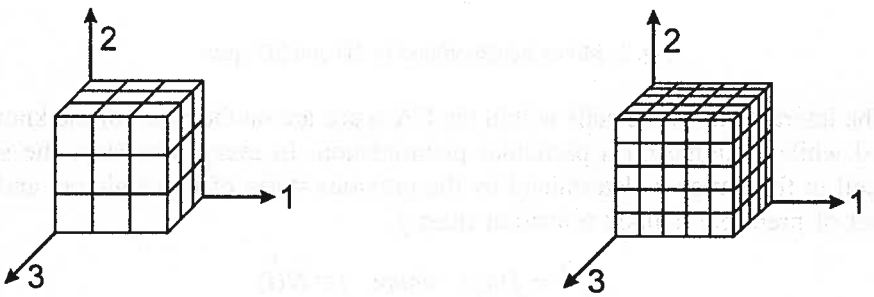

Fig. 2. Ductile CA space and brittle CA space

In the work [4] each cell in the ductile and brittle spaces is described by several state variables. The most important one is the variable that refers to the state of a particular cell. It is assumed that in a ductile CA space, each cell can be in two different states: *alive* or *dead*. For this case, a proper transition rule which describes the real material behavior during deformation was defined to control the ductile fracture initiation and propagation. Changes between the states *alive* and *dead* are due to equation:

$$\Upsilon_{m(D)}(t_{i+1}) = \begin{cases} alive \Leftrightarrow \beta_m(t_{i+1}) < \beta \\ dead \end{cases}, \tag{2}$$

where: $\Upsilon_{m(D)}(t_{i+1})$ — state of the m^{th} cell from the ductile space at the $t+1$ time step, β — is a damaged variable calculated from the Rousselier model describing the ductile fracture [4], t — time step.

The same analysis was performed for the *brittle* CA space; however, situation of this CA space is more complex. Each cell in the automata is described by four different states: *alive, aliveC, deadD, deadB*. AliveC is a special cell containing crack carbide. It is assumed that a cell in the state AliveC is a precursor of the initiation of the brittle crack in the material. State deadB refers to the selected cell, which died according

to the brittle transition rules (3), and deadD represents a cell that died according to the ductile transition rules (2). Those states are related to the mapping operations, which take place during calculations and are used for information exchange between *brittle* and ductile CA spaces. The transitions among the states in brittle CA space are controlled by a set of transition rules defined as:

$$\Upsilon_{m(B)}(t_{i+1}) = \begin{cases} deadB \Leftrightarrow A \\ \\ \text{where } A \in \end{cases} \begin{matrix} \sigma_I^m(t_i) > \sigma_F^m \wedge \{(\Upsilon_{m(B)}(t_i) = aliveC) \vee \\ \left(\begin{bmatrix} \Upsilon_{l(B)}^m(t_i) = deadB \vee \\ \Upsilon_{l(B)}^m(t_i) = deadD \end{bmatrix} \wedge \left|\alpha^m - \alpha^l\right| < \theta_F \right)\}, \\ \\ \Upsilon_{m(B)}(t_i) \end{matrix} \quad (3)$$

where: $\Upsilon_{m(B)}(t_{i+1})$ — state of the m^{th} cell from the brittle space at the t_{i+1} time step, σ_I — maximum value of the principal stress, σ_F — fracture stress, α — disorientation angle, Θ_F — critical value of the disorientation angle.

In [4] cellular automata spaces are connected to the single Gauss point in each 3D FE element via the ABAQUS user defined VUMAT procedure. From the FE solver, information about stress and strain is taken into account by cellular automata. Information about those macroscopic parameters is distributed along the CA spaces, and the transition rules (2) and (3) operate during each time step. As a result of calculations in the CA spaces, information about brittle and ductile fracture propagation is given to the FE solver according to the FE-CA transition rule. The transition rule between FE solver and CA solver is defined as follows: whenever a specific part of the dead cell in one of the CA spaces exceeds a declared critical value, then a particular FE element is removed from the FE mesh during further calculations in the next time step. A full description of this CAFE model can be found in [4]. Typical results obtained from this model are shown in Figures 3. The major advantage of this approach is a

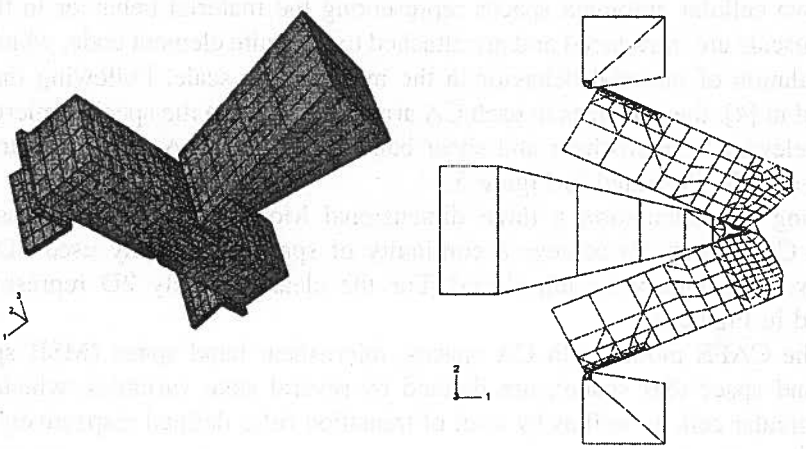

Fig. 3. Initial mesh before deformation in the Charpy test and final result of simulation obtained after deformation [4]

significant reduction in the computing time, when compared to the conventional FE model, which is attributed to the reduction in the number of FE elements.

Based on the multi scale idea proposed by Shterenlikht in [4], a 3D multi scale CAFE model of the formation of micro shear bands and shear bands is being developed. The initial results achieved from this model are presented in the next section.

3.1. CAFE model for strain localization

The problem of strain localization in material during deformation has been investigated by scientists for over thirty years. A huge effort has been made to study experimentally and theoretically shear band propagation during various kinds of deformation. 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 [2, 10]. However, there is still a lack of proper efficient numerical model, which accounts for influence of the formation of shear bands, and which can properly describe the material behavior in the FE simulation. Several attempts have been made to develop such a model [11, 12, 13], but the major disadvantage of these models is lack of flexibility and lack of possibility of generalization, which leads to difficulties with accurate description of the various forming operations.

All mentioned above facts are the reason of continuous search for the alternative approach to describe strain localization phenomena. Primary research performed by the authors has shown that the multi scale CAFE method should be an efficient method in this field. This model is a real multi scale approach including phenomena, which take place in different scales in the material, such as initiation and development of the micro and macro shear bands during various forming processes. Those two particular phenomena occur in the two different scales in the material: microshear bands initiate in the microscale, while shear bands appear in the mezoscale. According to these two scales, two cellular automata spaces representing the material behavior in the micro- and mezoscale are introduced and are attached to the finite element code, which handles the calculation of material behavior in the macroscopic scale. Following the concept presented in [4], the cell sizes in each CA array are linked to the specific microstructure feature relevant to microshear and shear bands phenomena. A schematic draft of the CAFE model is illustrated in Figure 5.

During the calculation a three dimensional Moore neighborhood was selected for both CA spaces. To achieve a continuity of space, commonly used 3D periodic boundary conditions were introduced. For the clearance only 2D representation is presented in Figure 4.

In the CAFE model both CA spaces, microshear band space (MSB space) and shear band space (SB space), are defined by several state variables, which describe each particular cell, as well as by a set of transition rules defined respectively for those spaces.

Internal variables describing state, rotation angle, and values necessary to initiate a hard and easy slip system in the material were introduced to the MSB space. A

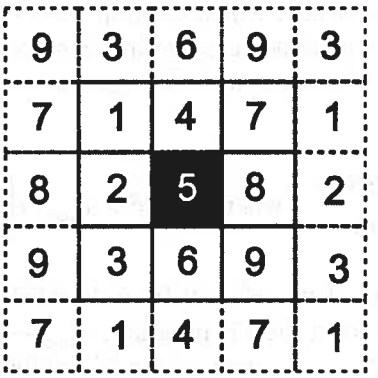

Fig. 4. Periodical boundary condition in 2D case

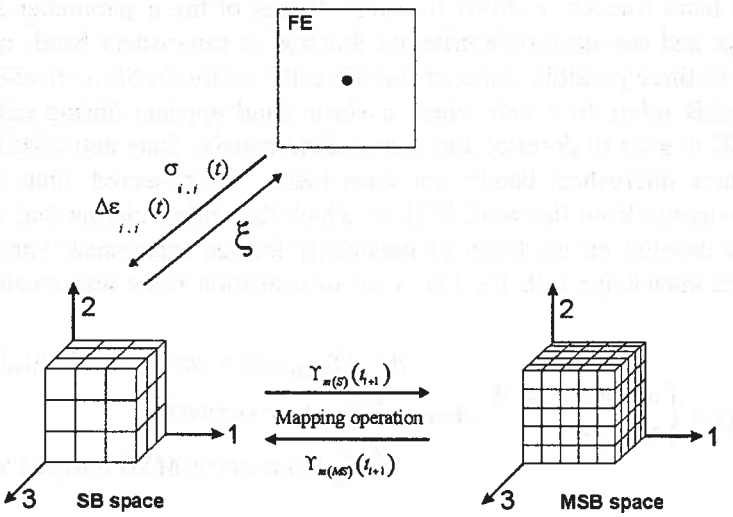

Fig. 5. Schema of the information flow between macro-, mezo- and microscale of the CAFE model. $\sigma_{i,j}$ — represent stress tensor, $\Delta_{\varepsilon_{i,j}}$ — represents strain increment, and Υ_m — represents the state of a selected m cell

particular MSB cell can be in two possible states – *nonactiveMSB* and *activeMSB*. A state activeMSB indicates that microshear bands development is taking place in this cell, while a nonactiveMSB refers to the surrounding matrix. Critical values of the variables describing stresses are generated for each MSB cell using the right hand side of the gauss function at the beginning of the deformation process. Transition rules controlling changes between two states in MSB space are defined basing on experimental knowledge [10, 14]. The author of [14] claims that initiation of the microshear bands is due to the occurrence of *slip domains* along the existing slip lines in the deformed material. Rotation of those domains and their development lead to

initiation of the micro shear bands, which develop most of the time in one particular grain, or in some cases in several adjacent grains. Similar observations were made in work [15]. Transition rules which provide a change from nonactiveMSB to activeMSB state are described by:

$$\mathrm{Y}_{m(MSB)}(t_{i+1}) = \begin{cases} activeMSB \Leftrightarrow A \\ \mathrm{Y}_{m(MSB)}(t_i) \end{cases} \text{where } A = (\delta > \tau^*_{\max}) \vee \begin{pmatrix} \mathrm{Y}_{l(MSB)} = activeMSB \wedge \\ \theta^{rot}_m - \theta^{rot}_l > \theta \end{pmatrix}, \tag{4}$$

where: $\mathrm{Y}_{m(MSB)}(t_{i+1})$ — state of the m^{th} cell from the MSB space at the t_{i+1} time step, σ — stress value achieved form the FE program, $\tau^*_{\max}$ — critical value for initiation of the hard slip system, $\mathrm{Y}^m_{l(MSB)}$ — state of the l^{th} neighbor of the m^{th} cell from the MSB space, θ — rotation angle.

Similar analysis is performed for the SB space. State variables and transition rules are defined as follows. Each cell is described by the variable representing state and microshear band fracture α (MSB fracture). Values of the α parameter are within the range <0, 1> and are used to describe the fraction of microshear bands in the SB cell. That leads to three possible states of the SB cells: *nonactiveSB, activeSB, activeMSB.* State activeSB refers to a cell where a shear band appears during calculation, and nonactiveSB is used to describe the surrounding matrix. State activeMSB refers to an SB cell where microshear bands, not shear bands, are observed. State activeMSB is a natural outcome from the work [10], in which the author claims that shear banding phenomena develop on the basin of previously formed microshear bands. Basing on the supplied knowledge [10, 13, 14], a set of transition rules was created for the SB space:

$$Y_{m(SB)}(t_{i+1}) = \begin{cases} activeSB \Leftrightarrow A \\ Y_{m(SB)}(t_i) \end{cases} \text{where } \begin{matrix} A = (Y_{m(SB)}(t_i) = activeMSB \wedge \alpha_m(t_i) > \alpha_{cr}) \\ \vee \left(Y^m_{l(SB)}(t_i) = activeSB\right) \\ \vee \left(Y^m_{l(SB)}(t_i) = activeMSB \wedge \alpha_m(t_i) > \alpha_{cr}\right), \end{matrix} \tag{5}$$

where: $Y_{m(SB)}(t_{i+1})$ — state of the m^{th} cell from the SB space at the t_{i+1} time step, $Y^m_{l(SB)}$ — state of the l^{th} neighbor of the m^{th} cell from the MSB space.

Information about the occurrence of microshear and shear bands is exchanged between the CA spaces during each time step, according to the defined mapping operations. Flow of the information between the scales goes in both directions, from macroscale to mezoscale and microscale as well as from microscale and mezoscale to macroscale. In each time increment, information about stress tensor is sent from the finite element solver to the MSB space, where development of microshear bands is calculated according to (4). After exchange of information between CA spaces, transition rules for the SB space (5) are introduced, and a propagation of the shear bands is modeled. Based on the information supplied by CA spaces, an equivalent stress σ^{CA}_p is calculated and is used to obtain correction coefficient ξ:

$$\xi = \frac{\sigma_p^{CA}}{\sigma_p^{FE}}. \tag{6}$$

This coefficient is sent to the FE program and is used for modifying the flow curve in the next step of FE calculations:

$$\sigma_p = \xi \cdot f(\varepsilon, \dot{\varepsilon}, T), \tag{7}$$

where: σ_p — equivalent stress, ξ — correction coefficient, ε — strain, $\dot{\varepsilon}$ — strain rate and T — temperature.
A schematic illustration of information flow in the CAFE model is shown in Figure 5.

4. Results

Primary calculations using the CAFE model for strain localization were performed for the simple compression in channel die test. During the calculation, 3200 gauss points were taken into consideration. FORGE 2 code was used in simulations. For each FE gauss point, two CA spaces were attached. During the first step, calculations were performed using the FE approach with conventional flow stress model, and during the second step comparison was made with the results obtained from the CAFE model (Figure 6). The CAFE model is based on the commercial FE FORGE 2 program and a CA code developed by the author.

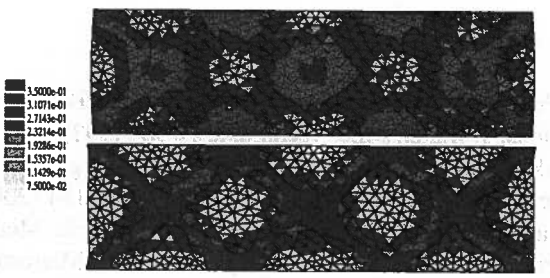

Fig. 6. Strain distribution results during the channel die tests achieved from the conventional FE model (top) and developed CAFE model (bottom)

It is clearly seen in Figure 6 that a strain localization in the band appears when the CAFE approach is applied. This is due to development of the microshear and shear bands in the micro and mezoscale, respectively, during the deformation process.

5. Conclusions

To sum up the results presented in this paper it should be concluded that:

- The CAFE approach is a full multiscale model, which is able to perform calculations in different scales in materials from micro to macroscale. It is possible to include stochastic phenomena, which take place during deformation, what makes this method a very powerful investigative tool.
- Earlier application of the CAFE approach by the authors to model crack propagation [16], as well as present work on modeling micro shear and shear bands propagation, proved very good predictive capabilities of this technique.
- Primary results achieved from the strain localization CAFE model replicate qualitatively realistic material behavior. The general form of the developed model, which does not constrain application of the model to particular tests or particular processes and allows simulations of any metal forming process, is the main advantage of this approach.
- Further work should focus on quantitative validation of the CAFE micro shear band model by comparing the results with the experimental data. Further improvement of the model will be conducted as well.

Acknowledgements

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