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MULTISCALE MODELING OF MICROSTRUCTURE AND MACROSCOPIC PROPERTIES IN THIXOFORMING PROCESS USING CELLULAR AUTOMATION TECHNIQUE

MODELOWANIE WIELOSKALOWE MIKROSTRUKTURY I WŁASNOŚCI MAKROSKOPOWYCH MATERIAŁU W PROCESIE TIXOFORMINGU Z ZASTOSOWANIEM AUTOMATÓW KOMÓRKOWYCH

The thixotropy phenomenon is strongly connected with the change of viscosity in time, while the shear rate and temperature are constant. One of the most important challenges in computer modeling of the materials that show such behavior is the proper description of microstructure development. The changes of microstructure during thixoforming processes are crucial to material properties, such as viscosity. Due to different scales of the models, the simultaneous modeling of microstructure development and viscosity property is still difficult. Therefore, the application of multiscale methods may provide the solution of the discussed problem. In this paper the multiscale model is proposed. The cellular automaton (CA) technique is used as microscale model. The main advantage of CA is ability to modeling of global behavior of the system on the basis of local interactions. In this paper the CA technique was applied for modeling of viscosity change and microstructural behavior of thixoformed material. The macroscale model is based on FEM solution of Navier-Stockes equation. The micro- and macroscale models are coupled using CAFE approach.

Keywords: multiscale modeling, thixotropy effect, thixoforming, semi-solid state, cellular automata

Zjawisko tiksotropii polega na zmianie lepkości cieczy przy ustalonej prędkości ścinania i temperaturze. W komputerowym modelowaniu zachowania się materiału wykazującego właściwości tiksotropowe (w tym stopów wykorzystywanych w procesach tiksoformingu), jednym z ważniejszych zagadnień jest poprawne opisanie zmian mikrostruktury w czasie. Zmiany te w sposób krytyczny oddziałują na własności makroskopowe materiału, w tym przede wszystkim lepkość. Równoczesne modelowanie zmian mikrostruktury i efektów makroskopowych jest utrudnione przede wszystkim ze względu na różnicę skal obu tych procesów. Rozwiązaniem tych trudności może być zastosowanie metod modelowania wielo-

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skalowego. W rozważanym przypadku modelowanie przeprowadzono bazując na połączenia układów równań różniczkowych cząstkowych (makroskala) oraz rozwiązań w skali mikro, wykorzystujących automaty komórkowe. Podstawową zaletą automatów komórkowych jest wykorzystywanie zależności lokalnych do modelowania globalnego zachowania systemu. W niniejszej pracy automaty komórkowe zastosowano jako model zachowania się mikrostruktury oraz zmian lepkości materiału (traktowanego jako ciecz nienewtonowska), poddawanego procesowi tiksoformowania. Obliczenia w skala makro i mikro połączone zostały w oparciu o metodologię CAFE (Cellular Automata Finite Element), integrującą automaty komórkowe z metodą elementów skończonych.

1. Introduction

The advantages of the semi-solid metal forming have caused the significant interests in this process in recent years [1]. In comparison with conventional casting or solid-state forming processes like forging or stamping, the semi-solid processes offer several advantages such as prevention of macrosegregation and porosity, relatively low forming temperatures (in comparison with casting) and lower forces (in comparison with the forging processes). One of the most interesting methods of semi-solid forming is thixoforming. This process depends strongly on specific microstructure, which must consist of solid metal spheroids in liquid matrix [2]. The alloys with proper microstructure and temperature can be formed with extremely low forces, even could be cut with a knife. The material in this state could be treated as viscous fluid. In short time of deformation the alloy behave as shear thinning liquid while in longer times the thixotropy effect becomes significant [3].

The thixoforming processes are constrained by very narrow range of temperatures. The difference between the highest and the lowest temperature could be only a few degrees. High sensitivity of the alloy viscosity with respect to temperature makes the material flow very complicated. The possibility of numerical modeling is essential for proper process development and industrial application. The macroscopic models of metal flow in short time intervals (without thixotropy effect) are well known and commercially employed [4]. However, for longer time intervals, when thixotropy effects become significant, these models are not sufficient. The construction of the models of thixotropy effect is not a trivial task. Although examined for many years, the mechanism of thixotropy in metals is still not very well recognized [5, 6]. The models of microstructure behavior during thixoforming, which were developed during recent years, are mainly based on thermodynamical equations, stochastic models or the combinations of them [7, 8, 9]. The numerical analysis of the primary microstructure development and the models of the influence of deformation are also difficult. The efforts are made to link the microstructural information and the macroscopic conditions of the process, such as viscosity, temperature and shear rates or the geometry of the sample. The models based on cellular automaton technique provide new possibilities in this field [10]. The objectives of this work are twofold. The first one is evaluation

of the applicability of the CA method to describe the behavior of semi-solid materials. The second aim is connection between CA model and FEM method.

Usually, the microstructure models are coupled with macroscopic modeling, based on finite element (FEM), finite difference (FDM), or finite volumes (FVM) method. Coupling of the micro- and macroscale models faces numerous obstacles, for both numerical and theoretical reasons. One of the methodologies of multiscale modeling is combination of cellular automata (CA) with finite elements (FE). This approach is known as CAFE methodology [11].

Application of this methodology to thixoforming is the main objective of this paper. The simulation of material test was chosen for the case study as an example. This test is commonly used for determination of properties for materials that exhibit the thixotropy effect. The CA model written in C++ was developed and linked with the commercial FEM code ADINA-F®. The results of CAFE computation are presented and discussed.

2. Model

2.1. CA overview

The cellular automaton approach was originally developed in early 60th of the last century for simulations of discrete, complex dynamic systems. One of the most famous researchers of computer science, John von Neumann, is considered as originator of the CA idea [12]. During the few last decades, the cellular automaton technique has become very powerful investigative tool [13]. The methodology of the CA simulations is briefly presented in [14]. The examples of application of CA method in the area of material science include the modeling of static [15] and dynamic recrystallization [16, 17], predicting the mechanical behavior of two-phase materials [18] and solidification processes [10].

The main idea of the cellular automaton technique is to divide a specific part of the material into the discrete lattice of the cells in required number of dimensions. Each cell is called *cellular automaton*, while the lattice of the cells is known as *cellular automata space*. Each cell in this space is surrounded by its neighbors. The common approaches for the 2-D CA modeling are Moore's and von Neumann's neighborhoods. The interactions between cells within the neighborhood are determined by a set of transition rules Ω. In the present paper, the hexagonal definition of neighborhood was chosen as the most appropriate.

In every time step, the state of each cell in the CA space is determined by the previous states of its neighbors and itself, according to the arbitrary declared transition rules. The transition of state γ of (i, j) cell is defined as follows:

$$\gamma_{i,j}^{t+1} = F(\gamma_{i,j}^{t}, \Lambda_{\gamma(i,j)}^{t}), \tag{1}$$

where t is time step number, F is the rule that belongs to the set of rules Ω and $\Lambda_{\gamma(i,j)}$ is a set of neighbors of (i, j) cell.

In the case of hexagonal neighborhood the transition of state dependency is expressed with regard to neighbors' lattice orientation (Figure 1):

$$\gamma_{i,j}^{t+1} = F(\gamma_{i,j}^{t}, \gamma_{i-1,j-1}^{t}, \gamma_{i-1,j}^{t}, \gamma_{i,j-1}^{t}, \gamma_{i,j+1}^{t}, \gamma_{i+1,j-1}^{t}, \gamma_{i+1,j}^{t}). \quad (2)$$

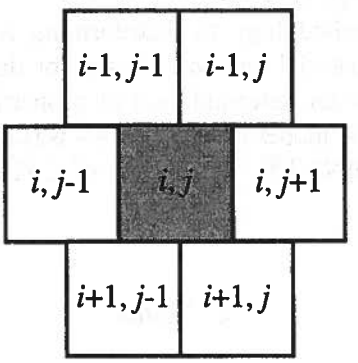

Fig. 1. The hexagonal neighborhood

In this paper the term of a *distant neighborhood* is introduced. This term refers to the group of cells that are connected by some properties. These cells are unable to affect each other, but are able to obtain some statistical information regarding the state of cells in distant neighborhood.

2.2. The CA model

The CA approach was applied in the two parts of the model. The first one was connected with generation of primary microstructure, while the second was used for modeling of rheology of the material. Both the models share the common parts, which are presented below.

It was assumed that each CA cell is characterized by finite state variable T and continuous variable E, which is interpreted as its capability to remain in state T. In addition to these variables, each cell may belong to two distant neighborhoods. Such a neighborhood is regarded as a group of cells that form a crystallite (grain) of the solid material. The state variable T represents four distinct states: liquid ("L"), solid ("S"), interface liquid-solid ("LS") and interface solid-solid ("SS"). The interpretation of the "SS" state is not quite obvious. It was assumed that crystallites never divide into subparts, however, they may agglomerate and form the meta-crystallites. The interfaces "SS" are intended to carry the information about the presence of the agglomerated crystallites. Moreover, the meta-crystallites may decompose into single crystallites by removal of interfaces "SS" that connect them together.

2.3. Generation of primary microstructure

The CA simulation of material rheology requires discrete image of initial microstructure. It should be pointed out that the image is not a direct representation of microstructure. Instead, it consists of the components, which have both morphological and geometrical meaning (such as liquid and solid phase) and some others, which have only morphological meaning (such as liquid- solid and solid-solid interfaces). The image of primary microstructure was generated using simplified normal grain growth algorithm. This algorithm is closely related to the method presented in [19] and based on the theory of Johnson-Mehl-Avrami-Kolmogorov. However, in the present work the generation of interfaces between phases and crystallites is introduced, accounting for the forming of meta-crystallites.

During each time step the amount of new nuclei is calculated and distributed randomly into CA space. The rate of nucleation is given by the formula:

$$\frac{dn}{dt} = \begin{cases} 0 & : \quad t < t_k \\ A & : \quad t \geqslant t_k \end{cases} \tag{3}$$

$$\mathrm{n}(0) = B$$

where A, B and t_k are the parameters and t is simulation time in arbitrary units.

The simulation is conducted until required fraction of solid f_s is reached:

$$f_s = \frac{N_S + N_{SS} + N_{LS}}{N_L}, \tag{4}$$

where N_S , N_{SS} , N_{LS} and N_L are numbers of cells in the state of "S", "SS", "LS" and "L", respectively. The typical result of the calculations is presented in Figure 2, which shows the microstructure generated using the grain growth algorithm (a) and a photo of real microstructure (b). The microstructural characterization can be measured by a shape factor F [20]:

$$F = \frac{8N_L^2}{3\pi f_s N_A}, \tag{5}$$

where $N_A = N_S + N_{SS} + N_{LS}$ is a number of structural units per area.

2.4. CA model of viscosity

The model of material viscosity aimed at taking into account the influence of shear rate. The expected outputs of the model should conform to the behaviour presented in Figure 3. Main idea behind the CA simulation of viscosity was inspired by the observation that various morphological phases are susceptible to the shear rate in different extent. Therefore, their representation in CA space depended on variable E, which could be interpreted as a capability to remain in state T. During each time step the variable E is modified according to the formula:

$$E^{t+1} = E^t + I(\dot{\gamma}, T) - O(T). \tag{6}$$

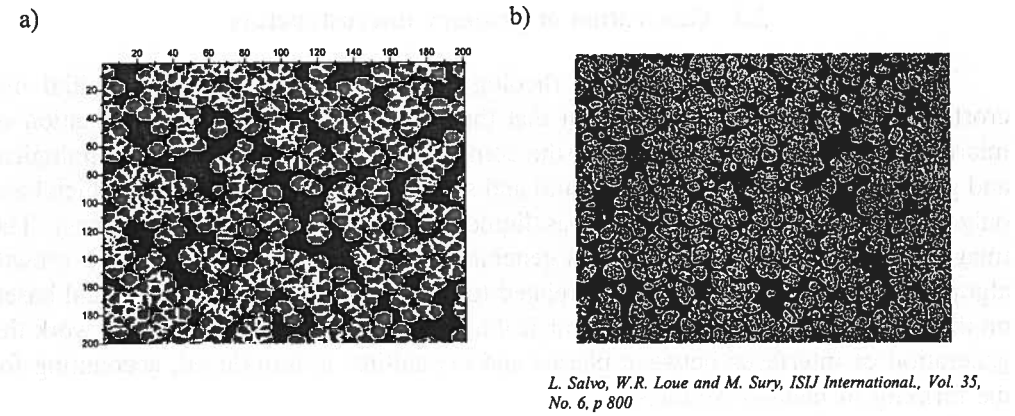

Fig. 2. (a) Typical distribution of state variable S at the lattice of cellular automata. The colour of the fields indicates the phase, to which the cell belongs: black — liquid, dark grey — solid, light grey — interface liquid-solid and white — interface solid-solid, (b) — photo of real microstructure, dark fields indicate liquid phase and grey fields are the solid crystallites

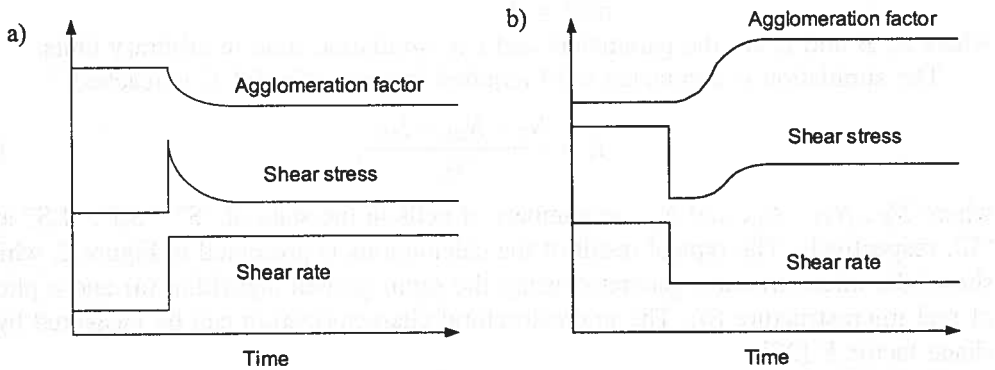

Fig. 3. The viscosity and degree of agglomeration as a function of time in the shear jump (a) and shear dump (b) conditions

The range of possible values of E was divided into four bands, considered as regions of stability of the phases (states) $R_T : \langle l_T, u_T \rangle$, where l_T and u_T are lower and upper bounds of state T stability, respectively.

If the variable E achieves the value, which is outside the region specific for the state T, the state of a cell could be changed. However, the conditions of state transition are more complex and also depend on the state of the neighbors and distant neighbors. The most general transition rules are as follows:

- The cell can change the state T if and only if the variable E is outside the region of stability R_T.

- The cell in state "S" can turn into interface "LS" if it has a neighbor in state "LS".
- If the cell in state "S" has a neighbor in state "L", then the value of its variable E is changed to l_{LS}.
- If the cell in state "S" has a neighbor that belongs to different crystallite (distant neighborhood) then it changes to the state "SS" and joins also that crystallite.
- The cell in state "SS" can turn into interface "LS".
- The cell in state "L" can change state to "LS" if it has a neighbor in state "LS" or "S".

The rules presented above are sufficient to describe the agglomeration and breakage of meta- crystallites and the movement, growth and shrinkage of crystallites. However, the preliminary computational tests have shown that the model tends to simultaneous "waves" of state transitions. In order to lessen this unfavorable and unrealistic behavior, the probabilistic factor was introduced to some of the transition rules. It was supposed that the thermodynamic equations for description of transition from liquid to solid would be more accurate. However, since the model would become much more complicated, that modification would entail significant increase of computational cost.

The form factor (5) was used as a measure of microstructure morphology. The viscosity of material was given as a function of F:

$$\eta = aF^{-1} + b, \tag{7}$$

where a, b are parameters. This model describes only the shear–thinning effect. The proper determination of viscosity on the basis of microstructure state or state changes still presents difficulties due to the lack of reliable experimental results in this field.

2.5. FEM model

Couette type viscometer had been chosen as an experiment for testing the model Figure 4. In this type of the instrument, the liquid between two coaxial cylinders remains in laminar flow with constant shear rate for an arbitrarily long time. Rapid rotation speed changes generate shear jump or shear drop conditions. Due to lack of access to the experimental device, simulations and verification have been based on the data found in literature [21, 22, 23]. The FEM model of Couette viscometer has been developed in both two- and three- dimensional versions. ADINA-F® commercial code has been employed. The viscous, incompressible, non-Newtonian fluid has been used as material model. Isothermal conditions were assumed. The preliminary calculations were performed with use of the power law (Ostwald-de Waele) model of liquid material. These calculations confirmed that the proper assumptions for geometry and boundary condition were applied. The distribution of velocity in cross-section of sheared fluid was computed for 2D and 3D models. The model was capable to take into account both the shear jump and shear drop conditions.

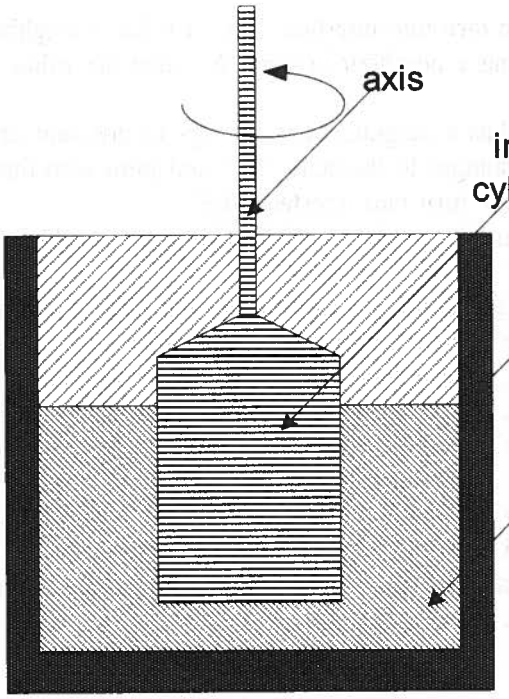

Fig. 4. The Couette type viscometer

2.6. CAFE model

The connection between FE and CA models was introduced on the basis of CAFE methodology. The interaction between the levels of the model is shown in Figure 5. Regular finite elements mesh has been introduced. Due to axisymmetrical veloc-

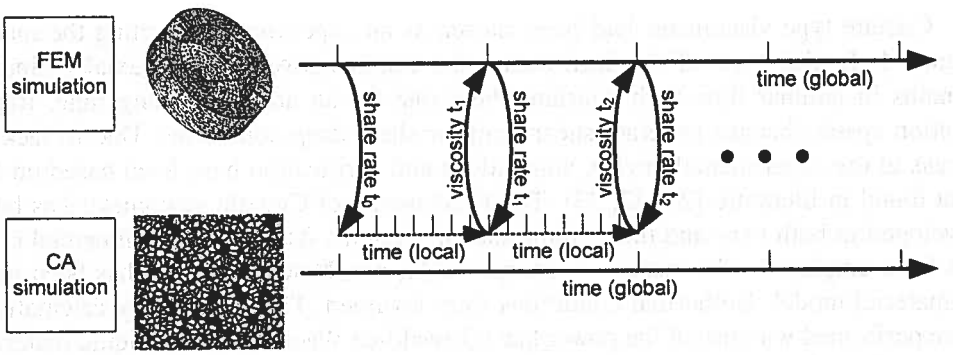

Fig. 5. The schematic representation of coupling FEM and CA simulations

ity distribution, shear conditions were varied only in the radial direction and were maintained constant in the circular direction. It was assumed that viscosity could be

computed only for one node in each coaxial layer of nodes and applied in each node in this layer (Figure 6).

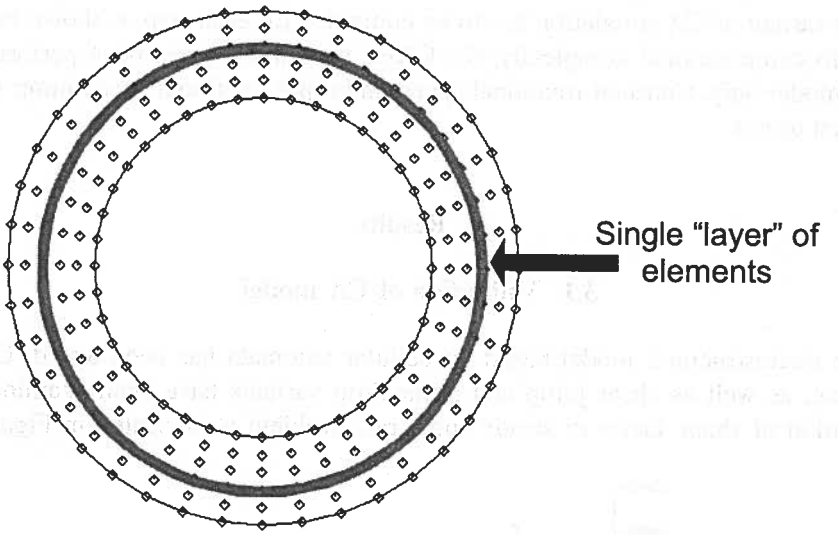

Fig. 6. "Layer" of finite element nodes in the viscometer model

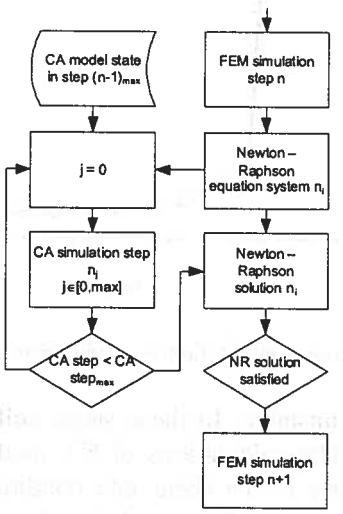

Fig. 7. The algorithm of coupled CAFE method. The CA simulation is called in consecutive steps of Newton-Raphson solver

Equations system generated in ADINA code has been resolved with explicit Newton-Raphson algorithm. For the selected nodes (one in each layer), the CA simulation has been performed (Figure 7). As it was assumed, CA simulation is continuous during

whole FE simulation time. In each FE step, a number of CA simulation steps are computed with border conditions inherited from corresponding step of FE model. A few Newton-Raphson algorithm iterative solutions are checked for each FE model step. Another variant of CA simulation has to be computed for each step as shown in Figure 7. Due to computational complexity, the CAFE simulations have been performed for the 2D model only. Constant rotational speed and rapid rotational speed jump variants have been tested.

3. Results

3.1. Validation of CA model

The mictostructural model based on cellular automata has been tested. Constant shear rate, as well as shear jump and shear drop variants have been examined. The stabilization of shape factor in steady shear rate problem is presented in Figure 8. In

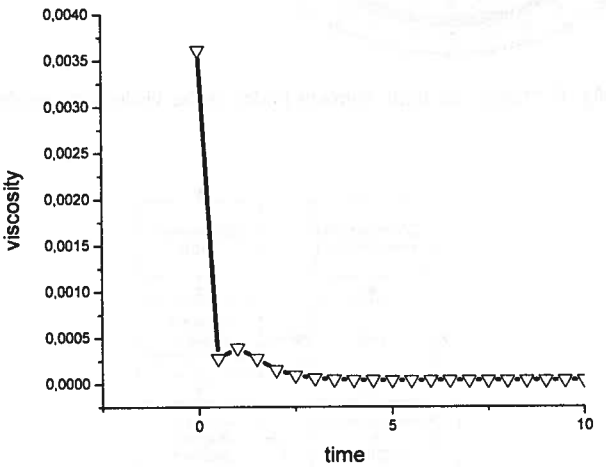

Fig. 8. Viscosity stabilization in steady shear rate problem

initial steps the factor F is unstable. In these steps, cellular automata space is fitted for given shear rate value. The calculations of CA model showed that the image of microstructure adapts properly to the shear rate condition. When the microstructure is appropriate for used shear rate, CA simulation becomes stable. Figure 9 shows comparison of experimental viscosity values as a function of shear rate for A356 aluminum alloy presented by Kim and Kang [24] with results obtained from CA simulation.

Significant effect of thixotropy materials is lack of sensitivity of steady (after stabilization) viscosity which respect to history changes. The results obtained for shear jump and shear drop are shown in Figure 10. These results confirm the proper behavior

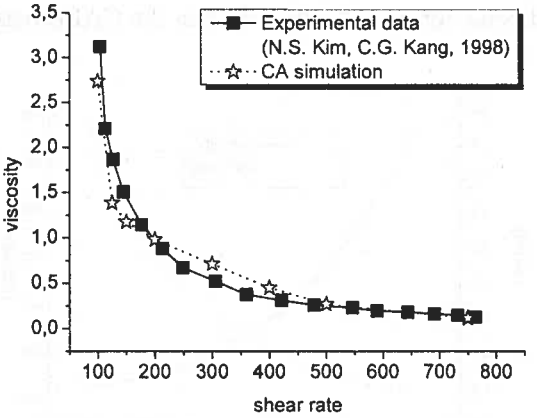

Fig. 9. Comparison of experimental and computed viscosities as function of the shear rate

of CA model. The response of the model shows that the history of the process is accounted. Moreover, the path of the process affects viscosity and is dependent on shear rate.

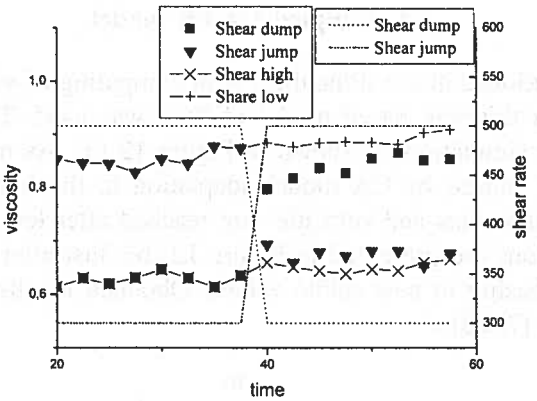

Fig. 10. The response of the CA simulation on the shear jump and drop. Full symbols present viscosity changes during the shear dump (dot line) and jump (dash-dot line). "X" and "+" symbols presents viscosity in constant higher (X) and lower (+) shear rate

3.2. FEM model

Figure 11 shows the velocity and viscosity distribution in pure FEM model of Couette system viscometer. The results are consistent with our expectations — the velocity decreases with radius growth while the viscosity decreases with growth of the velocity derivative. In case of shear jump, viscosities for the whole domain are lower after jump, when velocities differences are higher. These results are consistent with

shear-thinning liquid behavior. It was expected that the CAFE based model would give similar solutions.

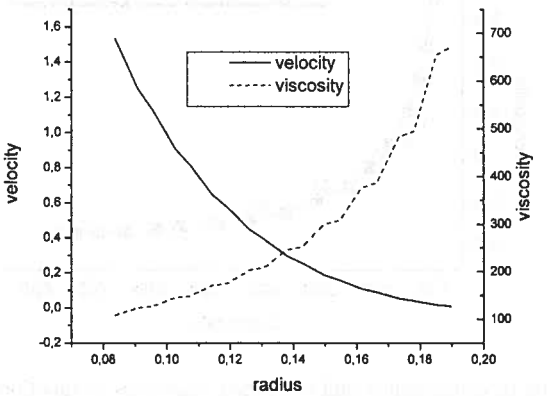

Fig. 11. Velocity and viscosity distribution along the radius in the FEM model of the Couette system Viscometer. The viscosity is calculated acording to the Ostwald-de Waele power-law

3.3. Coupled CA-FE model

Because of mentioned above difficulties with computing of viscosity in thixotropy case, classical shear thinning based model of fluid was used. The average viscosity in steady shear rate simulations is shown in Figure 12 (a). As mentioned above, initial fluctuations are caused by CA model adaptation to the boundary conditions of shear rate. Stable viscosities and velocities are reached after few steps. The results of shear jump simulations are presented in Figure 12 (b). Just after shear jump, average viscosities are decreasing to new stable values. Obtained results are coincident with experimental works [7, 23].

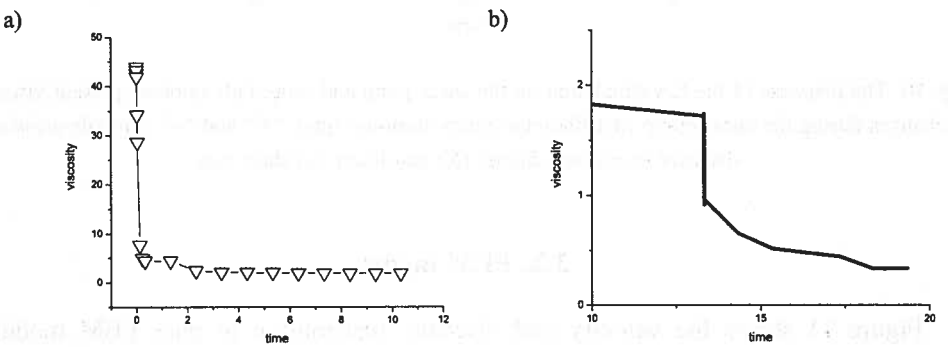

Fig. 12. Average viscosity in steady shear rate simulations. Stabilization of the viscosity daring constant shear rate (a) and viscosity dump for the jump of the shear rate (b)

4. Discussion and conclusions

CA models for shear-thinning and thixotropic fluid have been designed. Agglomeration factor for both models could be efficiently predicted in steady shear rate as well as in the shear jump/dump case. Method for viscosity computation based on microstructure CA model simulation has been developed. CAFE platform, based on commercial FEM code and own CA code has been worked out.

The presented results proved that CAFE methodology could be successfully used for multiscale modeling of viscous fluids flow. When CAFE methodology is employed, more information concerning microstructure behavior is collected. Especially the data regarding the history of the process could be stored and presumed during computation, what is impossible or very difficult in classical methods (FEM, FDM, FVM). Following, the history dependent effects, such as thixotropy, can be modeled. The CAFE methodology applications allow increase of the FE mesh size with maintaining accuracy of the microstructure modeling. Computation time could be decreased accordingly. Since it is not possible to employ CA model in each FE node, the proper simulation design is essential.

The main problem in simulations is difficulty with binding degree of deglomeration (shape factor) changes with viscosity. Proper methods of viscosity computing are essential for dynamic effects modeling in macroscale during thixoforming processes. The selection of transition rules also requires further research. However, the idea of two-variable (T,E) cellular automata seems to provide satisfactory results. The physical explanation of the E variable is still unclear. It may be concluded that introduction of such a concept gives acceptable results, at least at this level of simulation. Keeping in mind that CA simulation is intended to be descriptive models, the introduction of advanced thermodynamics into the CA model would make it computationally unfeasible. The further research is planned, concerning experimental verification of microstructural effects in thixoformed metal alloy.

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