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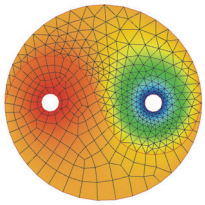

CONCURRENT AND UPSCALING METHODS IN MULTI SCALE MODELLING – CASE STUDIES

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Abstract

Selected examples of applications of multi scale modeling in various areas of mechanics and materials science are presented in the paper. Advantages and disadvantages of these approaches are shown. Based on the literature review a classification of multi scale methods into two groups was pointed out. The first is upscaling group based on representative volume element. The second is concurrent group, where the method used to describe the fine scale is usually applied to a part of the whole domain of the solution. Detailed discussion of these two groups is based on the multi scale models developed by the Authors. The concurrent model is based on the combination of the molecular dynamic with the boundary element method and is applied to simulation of material failure. The upscaling model is called CAFE and is based on the combination of the cellular automata with the finite element method. Applications of this model to prediction strain localization in materials subjected to plastic deformation are also demonstrated in the paper.

Key words: multi scale modelling, cellular automata, atomic models, fracture, strain localization, micro shear bands

1. INTRODUCTION

The accuracy of numerical simulations of metal forming processes depends, to a large extent, on the appropriateness of the description of the material flow, as well as the mechanical and thermal boundary conditions. The former aspect is the topic of the present work. One of the challenges in simulations of thermo-mechanical processes is evaluation of the material flow parameters for various deformation conditions. The general procedure involves performing plastometric tests, such as compression or tension or torsion, and interpretation of the results of these tests, using preferably the inverse analysis (Szeliga et al., 2006). The main sources of errors, which further influence the accuracy of numerical simulations, are due to:

- Inaccuracies in the plastometric tests.
- Errors in the inverse analysis, particularly due to errors in evaluation of the friction conditions in the tests.
- Inability of the selected material model to describe the real behaviour of this material.

The general objectives of this paper are connected with the development of a procedure that will guarantee development of accurate and reliable material models. This paper is a continuation of an earlier publication (Pietrzyk et al., 2006), where critical analysis of experimental tests, application of a method for automatic interpretation of results of

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the tests and, finally, mathematical description of the measured properties, were presented. The advantages and limitations of various material models, including conventional models based on closed form equations, internal variable models and multi scale models, were also discussed. The present paper is focused on the third group of material models, that are based on multi scale analysis.

Multi scale modelling has recently become very popular in various disciplines. The number of applications of these models is increasing rapidly and the variety of approaches to multi scale problems is large. Therefore, there is a need for classification of the available methods and systematisation of their applications. Several papers dealing with these problems can be found in the literature, with that focused on multi scale modelling in material science (De Borst, 2007) of particular note. The general objective of the present work is to focus on plastic deformation of metals and application of multi scale models as constitutive laws in metal forming simulations. The particular objectives of the paper are twofold. A review of available multi scale material models is presented first with the goal to outline the wide variety of these approaches and highlight main distinctions between them. The particular emphasis is on the capabilities and limitations of the various methods. Finally, this is followed by detailed discussion focusing on particular case studies, that represent two main branches in multi scale models.

2. MULTI SCALE MODELLING METHODS

2.1. Motivation

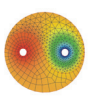
The development of reliable material models for metal forming simulations has been of interest to scientists for a number of years. A number of deterministic models, based either on closed form equations describing the flow stress dependence on external variables (Grosman, 1997), or on differential equations describing the evolution of internal variables (Estrin, 1996; Roucoules et al., 2003) have been published in the scientific literature. These models are commonly used in simulations for the majority of metal forming processes and give reasonably accurate results. These models fail, however, to describe the material behaviour when some special conditions of deformation occur, eg. fast changes in the deformation conditions or a strong tendency to strain localization. The main problem is to realistically describe the phenomena occurring in materials at lower length scales under the above complex conditions of deformation and to incorporate this into the continuum based approaches. Beyond this, accounting for the influence of such phenomena as cracks, shear bands, Luders bands and Portevin-le-Chatelier bands in macro scale and such discontinuities as micro shear bands, grain boundaries, phase boundaries in the micro scale, become necessary when the model aims to predict the properties of the final products. Finally, several of these phenomena are stochastic in nature and their realistic description by deterministic models may be limited.

Thus, the search for models that account more accurately for micro scale and even nano scale phenomena has been the objective of research during last two or even three decades. The improvements in experimental techniques were major factors stimulating this research. New experimental techniques have made it possible to visualize physical processes and to measure relevant parameters at fine scales. Examples connected with new experimental equipment allowing research on mechanics of deformation are atomic force microscopy (AFM), nano indentation tests, computer tomography, electron back scattered diffraction (EBSD) etc. These techniques are supported by the established approaches such as scanning and transmission electron microscopy. The knowledge obtained about mechanisms of deformation from these experiments has been recently combined with the idea of multi scale modelling of materials to develop models with new predictive capabilities.

2.2. Classification of multi scale modelling methods

The modelling of discontinuities is now playing a more important role in analysis of material behaviour during plastic deformation. As mentioned above, the conventional material models are not amenable to capture of discontinuities. Accordingly, next to multi-physics phenomena and multi scale analysis, capture of these discontinuities is the third major challenge in contemporary computational mechanics of materials (De Borst, 2007). A fourth challenge constitutes the further development of computational methods to assess the probability of failure. The methods to cope with these challenges are usually classified into two groups: upscaling methods and concurrent multi scale computing (De Borst, 2007).

In the upscaling class of methods, constitutive models at higher scales are constructed from obser-



vations and models at lower, more elementary scales. The idea of the representative volume element is employed here. By a sophisticated interaction between experimental observations at different scales and numerical solutions of constitutive models at increasingly larger scales, physically based models and their parameters can be derived at the macro scale, see for example (Das et al., 2002). The methods of computational homogenisation, eg. (Mieche, 2003), are considered to belong to this group of methods.

In concurrent multi scale computing one strives to solve the problem simultaneously at several scales by an *a priori* decomposition. Two-scale methods, whereby the decomposition is made into coarse scale and fine scale, have been considered so far.

Both groups of methods have been intuitively used for decades. The solution of microstructure development equations in each Gauss integration point in the finite element (FE) model, and returning information regarding the flow stress accounting for microstructure, is a typical example of upscaling (Pietrzyk, 1990). An approach presented in (Hirt et al. 2007) is an example of concurrent computing. Recent years have, however, witnessed the rapid development of the multi scale methods in various areas of science and applications in deformation processes are particularly frequent. Various discrete methods have been applied to describe material behaviour at the micro and/or nano scales, eg. cellular automata (CA), molecular dynamics (MD), monte carlo (MC) methods. For example analysis of (Gawad & Pietrzyk 2007, Yazdipour et al. 2007) and (Rondanini et al. 2006; Yu & Esche 2005) can reveal differences in the application of CA and MC methods, respectively, to simulate recrystallization phenomena. Coupling between fine scale and coarse scale is now completed in a more systematic manner. Figure 1 shows the general idea of the distinction between upscaling models and concurrent multi scale computing.

In the concurrent multi scale computing the method used to describe the fine scale is applied to a part of the whole domain of the solution. It can be either the same method, which is used in the coarse scale, for example the FE method, or it can be one of the earlier mentioned discrete methods (CA, MC). In the former case the extended finite element (XFE) and the multi scale extended finite element (MS-XFE) methods are examples. In the XFE solution special elements capable to accommodate a discontinuity are introduced (Figure 2).

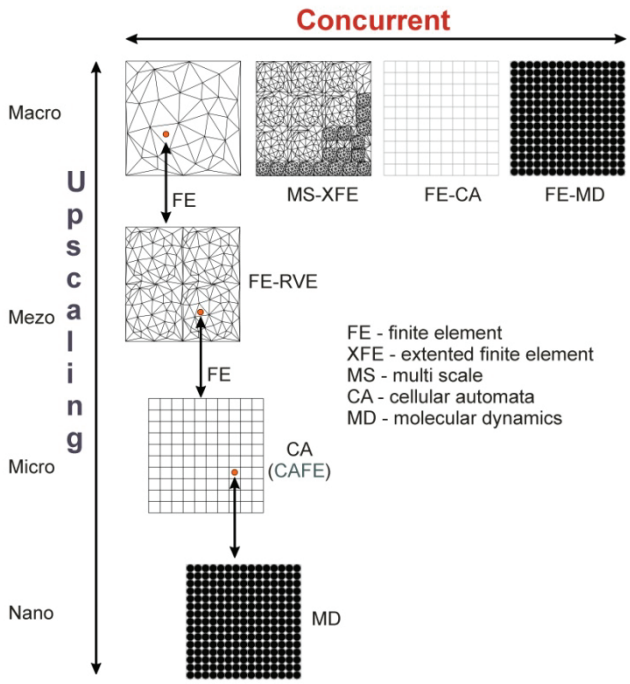


Fig. 1. The idea of distinction between upscaling models and concurrent multi scale computing.

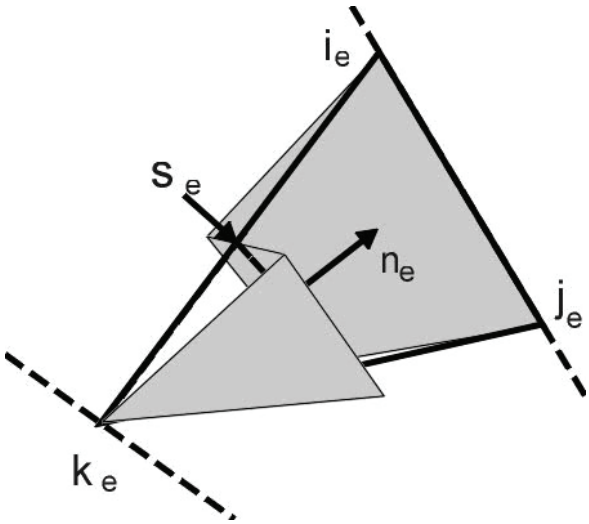


Fig. 2. Illustration of the finite element approximation of the unit jump function, which is the basis of the XFE approach (where: k_e, i_e, j_e nodes, S_e – discontinuity path, n_e – the normal vector to S_e).

In the MS-XFE method a very fine mesh is generated in the area of particular interest that is selected before simulation. The example is the area around the front of a crack propagation in a simulation of fracture, as shown in Figure 3 (Allix, 2006). The methods of mesh adaptation, eg. hp adaptation (Demkowicz et al., 2002; Paszyński et al., 2006), multi grid method (Dumett et al., 2002) and variational multi scale (VMS) methods (Volker et al. 2006) are also considered to belong to the concurrent multi scale computing group.

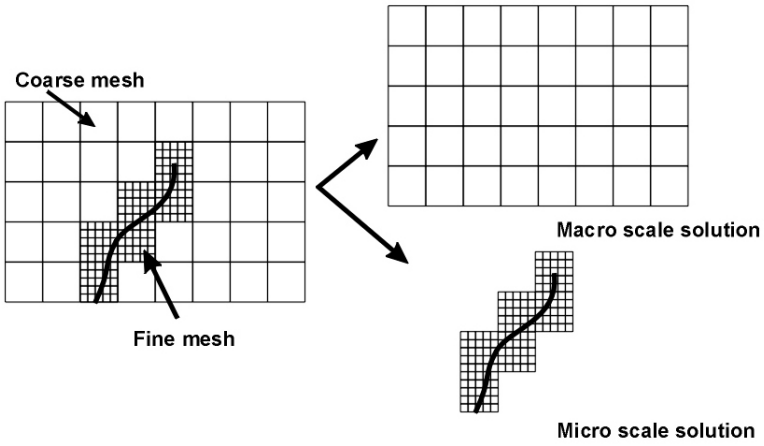


Fig. 3. Idea of MS-XFE scale decomposition.

An example of the upscaling method based only on the FE method is presented in (Milenin & Muskalski 2007). The two scale model based on the FE method combined with the representative volume element (RVE) approach is proposed to simulate the influence of colony composed of ferrite and cementite on the macroscopic behaviour during wire drawing. The deformation of the pearlitic colony and changes in orientation of cementite lamellas during the multi-pass drawing is investigated. The macro scale model uses a two dimensional rigid-plastic method that provides the boundary conditions for the micro scale model. To impose the boundary conditions on the grain boundary the penalty method is applied. As a result of the micro scale simulation the friction coefficient is modified in the macro scale solution. This work can be classified as conventional multi scale model based on the FE solution of the problem in two different scales within the up scaling group.

A large group of multi scale methods is represented by the multilevel models (i.e. Van Houte et al., 2006). Here parameters for the macro scale model are identified by the multilevel model. Usually multilevel models are composed of two or three levels i.e. (macro-meso scales or macro-meso-micro scales, respectively). The multi scale model was implemented in the finite element framework using the homogenization procedures to exchange information between scales all the way up to the macro scale. This approach is mainly based on the crystal plasticity models (Lamel Model, Advanced Lamel Model, Grain Interaction Model, Crystal Plasticity Model) that take into account interactions between particular grains as well as their rotations during deformation at the micro scale. In such an approach grains are usually represented by one finite element or in more advanced cases by many finite elements, which increases the computational time. This work can be classified as conventional multi scale model within the upscaling group.

However, not only is the FE method used to create multi scale approaches. The boundary element method (BEM) is also widely used e.g. (Sfantos & Alibadi, 2007). In that work a two scale model based on the combination of the macro BEM with the micro BEM as well as macro FE with micro BEM are considered for simulation of intergranular micro fracture in polycrystalline brittle materials. To investigate material behaviour at the lower scale a set of RVEs is assigned to the points. The attached RVEs represent grains of the microstructure in the infinitesimal neighbourhood of the macro scale points. The macro scale solution, related mainly to the stress and strain fields are treated as boundary conditions for the micro scale problem. The exchange of information is based on the averaging theorem (Nemat-Nasser, 1999). On the other hand the micro scale solution is used to update the constitutive laws at the macro scale when micro damage is possible. This eventually results in strain softening at the macro scale.

An interesting multi scale model based on the mesh free methods has been developed in (Missoum-Benziane et al., 2007), where a two scale approach using a constrained natural element method (CNEM) is applied to simulate linear elasticity problems. The model has the ability to take into account the microstructure changes and their influence on macroscopic behaviour. The analyzed domain is divided in two regions, a microscopic one that represents microstructure evolution in the entire macroscopic domain, and one called the complimentary domain that describes the macro scale (Figure 4).

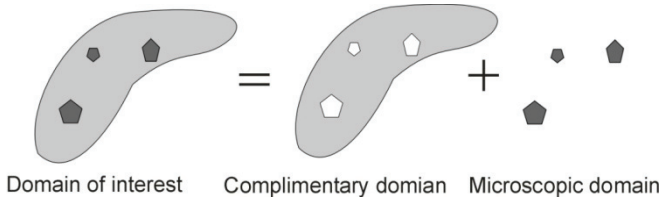


Fig. 4. Division of domain applied by (Missoum-Benziane et al., 2007).

The constitutive relations are defined only at the micro scale level and are then extended by the interpolation to the complimentary domain.

Despite large interest in conventional multi scale models based on eg. FE or BEM there has been a recent interest in the development of alternative methods that represent concurrent, as well as upscaling, approaches. For example, Rondanini et al. (2006) used the MC method to describe the growth of layers in the chemical vapor deposition (CVD) process. This solution is coupled with FE, which predicts the temperatures and stresses in the resulting multi layer coating. The interesting application in material science is presented in (Yu & Esche, 2005), where a multi scale model based on the FE with the MC pots method was used to simulate static recrystallization and grain growth during annealing. The FE method is used to simulate the macroscopic plastic deformation. The field variables obtained in the macro scale are then input data for the MC model for simulation of the microstructure evolution. In order to reduce the computational time the microstructure models based on MC are only considered in a few representative elements of the FE mesh. Information about the microstructural changes are finally sent back to the FE code, or are compared with the experimental results to optimize the process parameters. Another alternative model developed by Mrozek et al. (2007) uses the MD method coupled with the BEM to describe crack initiation and propagation. This approach will be described in detail in the following section. A very interesting method that is based on the molecular dynamics framework was developed in (Abraham et al., 1998), for the rapid brittle fracture of a silicon slab under uniaxial tension. The main idea of the approach is to divide a domain into three regions. The first is located away from the crack tip and is simulated by the continuum FE method. The second is located near the crack tip and is modelled by molecular dynamics, while the last region is located at the crack tip. This region is simulated using the tight binding (TB) method, which is a quantum method containing electronic information and is commonly used in the description of matter.

When the interface between continuum and molecular dynamic is considered all finite elements in this region are refined to match exactly with the atomic positions. Through these interfaces information exchange between two methods is performed which makes it also an example of the concurrent approach.

Another similar approach by (Tadmor et al., 1996), uses the multi scale quasicontinuum (QC) method to simulate macro scale nonlinear deformation of crystalline material again using molecular mechanics. In the method the material is divided into two main regions. The first is related with the surrounding material where no nonlinear behaviour is observed, and this region is simulated using only the finite element approach. The second region is related to nonlinear behaviour, where the molecular dynamics and finite element approaches coexist. To reduce computational time in the regions of small deformation atoms are segregated into two groups: non representative and representative. In this region the position of non representative atoms is interpolated based on the position of representative atoms that are positioned at nodes of the FE mesh (Figure 5). However, in the most interesting region, where we obtain larger deformation, the FE mesh is refined to match all atomic positions.

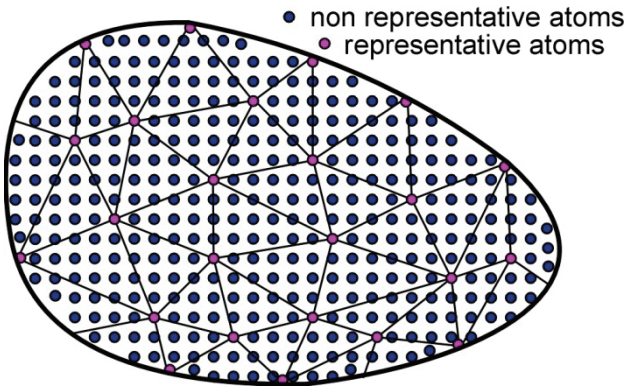


Fig. 5. Material division to non representative and representative atoms used in (Tadmor et al., 1996).

Another group of alternative methods is the CAFE approach based on the combination of the CA and FE methods. Four major directions of development of the CAFE approaches can be identified here. The first proposed by (Gandin et al., 1994), can be classified as a concurrent multi scale method. In this work (Gandin et al., 1994) the sample area is overlaid by the two separate meshes: FE and CA. The square CA space is defined to be more dense than the FE triangular mesh. A CAFE method is applied to model the development of dendritic structures during solidification. In this approach a differential equation describing the temperature field is solved using the FE model. However, a CA method was applied to model microstructure development and heat generation during solidification. This approach is still under further development (Gandin & Rappaz, 1996; Takatani et al., 1999; Thevoz & Gandin, 2001; Lee at al., 2004). A similar model for solidification simulations has also been applied by other authors (Quested & Greer, 2005; Vandyoussefi &

Greer, 2002). Another interesting work based on the previous CAFE model (Lee et al., 2004) is also related to solidification, in particular dealing with prediction of micro segregation and its influence upon micro porosity during the casting of automotive components. The micro scale approach is a combination of stochastic and deterministic methods such as CA and the finite difference (FD) method and deals with multi component diffusion in a three-phase system: liquid, solid, gas. During these micro scale simulations the nucleation and growth of grains and pores is calculated. The FE model provides information regarding heat transfer and fluid flow to the micro scale model. This model is partly similar to the work by Gandin (Gandin et al., 1994) and can also be classified as a concurrent method. Combination of the CA and FD method has also been applied to simulate the development of dendritic structures, but only at the micro scale (Yang et al., 2004). Application of the FD method to support CA calculations in the micro scale is also commonly used during phase transformation (Kumar et al., 1998; Zhang et al., 2003; Kundu et al., 2004). FD is applied to solve the diffusion equation while CA was usually used to track the state of particular cells in the domain to investigate the fraction transformed.

A second group represents the upscaling approaches, where separate cellular automata are attached to each particular gauss point in the FE mesh (Das et al., 2002, Shterenlikht & Howard 2006, Madej et al., 2007). The main advantage is a back propagation between methods in every time step, which increases the accuracy of computation. In the papers by (Das et al., 2002) a multi scale CAFE method was applied to model fracture phenomena occurring during various forming processes. The model predicts the microstructure development, as well as crack propagation in the surface layer during rolling operations. Microstructural features such as grain boundaries, other phase particles and grain interior are included during simulation in the CA spaces. The developed algorithm incorporates three major steps: development of the primary microstructure, flow of the macroscopic parameters obtained from the FE simulation to the CA mezo scale and, finally, back propagation of the parameters calculated in the CA spaces to the FE model.

This model (Das et al., 2002) was the motivation for the CAFE model created by Shterenlikht (Shterenlikht & Howard 2006). This approach describes propagation of the brittle and ductile fracture during a Charpy test. In this approach, two 3D cellular automata spaces are introduced. The first, called the ductile space, describes phenomena connected with ductile fracture, while the second one, termed the brittle space, describes phenomena connected with brittle fracture during the Charpy test. Because the sizes of brittle and ductile fractures differ, a different number and different dimensions of the CA cells are used in those CA spaces. The model then provides information about the cracks to the macro scale FE model. A further example of a CAFE model dealing with fracture can also be found in the work by Khvastunkov & Leggoe (2004).

Another interesting application of the multi scale CAFE approach is applied to simulate dynamic recrystallisation (DRX) (Gawad & Pietrzyk, 2007). Here there are three layers representing the macro, mezo and micro scales. The first layer is based on FE and provides the macroscopic description of the material. The constitutive law is based on the Levy-Mises flow rule, in which flow stress σ_f is the only material parameter. The second layer is a connection between the macroscopic and microscopic models, and includes calculation of σ_f, which is sent to the FE code. The local parameters, such as temperature and strain rate, are transferred in the opposite direction. The third layer, which is based on the CA calculations simulates the evolution of the microstructure and dislocation density.

Application of the CAFE model to simulate strain localization (Madej et al., 2007) in the material will be described as a case study in more detail in the following sections.

The third group of methods does not utilise back propagation and the flow of information is in one direction i.e. from the FE to CA models (Lan et al., 2005). Usually the area of the sample is limited to a few grains to reduce calculation time because several finite elements are applied to describe each particular grain. The amount of energy accumulated during deformation, as well as the grain crystallographic orientation, is obtained from the single crystal plasticity FE model and used as input data for the CA calculations of the austenite-ferrite phase transformation process after deformation. The detailed description of the CA model itself can be found in another work (Lan et al., 2004). These methods may be classified as concurrent approaches.

The final group of methods is related to various combinations of the CAFE method with other computational approaches such as Neuro Expert Cellular Automata Finite Element models (NESCAFE).

NESCAFE modelling is a very interesting approach dealing with hybrid microstructural models to take into account, in an explicit manner, development of microstructural features over various length scales. One of the examples of such an approach is a combination of Neuro- Fuzzy (nF) and Cellular Automata (CA) techniques attached to the FE code. The CA hold information concerning the material i.e. grain boundaries and grain interiors, subgrains, misorientation while the nF predicts the flow stress behaviour model based on this information (Das et al., 2007). Another model takes into account more microstructural details i.e. micro bands. The CA model describes grain interiors and grain boundaries and also the periodic function (φ). This function (φ) represents the spatial development of micro bands which depends on the initial orientation of CA cells. These hybrid methods are mainly classified as upscaling approaches.

Summarizing, it should be emphasized that a variety of possible multi scale approaches are commonly used. These approaches are distinguished as upscaling and concurrent multi scale computing but, in general, various continuum (FE, BE, natural element method) and discrete (CA, MC) methods can be used in both approaches. The distinction between the two groups of approaches is based on how the domain of the solution is handled. In the upscaling group of methods the coarse scale method covers the whole domain of the solution, and the lower scale methods are applied at selected points (the RVE idea) and they usually calculate the material parameters required in the constitutive law of the macro analysis method. In the concurrent multi scale computing approach various parts of the domain are covered by various methods. As shown above, all possible associations of the continuum methods and discrete methods are possible.

However, for full understanding of the differences between the concurrent and upscaling approaches the detailed case study is necessary. To provide this the two models developed by the authors will be discussed in depth in the following sections with particular emphasis on capabilities and limitations of these approaches.

3. CONCURRENT MULTI SCALE CALCULATIONS – CASE STUDY

Various continuum methods can be used to simulate the macro behaviour of materials. As mentioned in the concurrent multi scale calculations one method can be used for both the coarse and fine scales, or the macro scale method can be combined with the discrete methods (MC, CA, MD). In the former approach usually FE is able to replicate real phenomena that take place in the materials at different scales. This is the reason that various new versions of this method have recently been developed (XFE, MS-XFE) and are commonly used in the multi scale analysis. The latter case is considered as the case study in this paper. Finite and Boundary Methods are often applied to obtain complex description of material behaviour under loading and this method is considered in the following section of the paper. Thus, the continuum (FE/BEM) approach is used to describe model at the micro scale, and the molecular static is applied at the nano level.

3.1. Coupled Boundary and Finite Element Methods with Atomic Model

The multi scale algorithm based on the finite and boundary element methods (Burczynski, 1995) coupled with a discrete atomistic model is described in this section. Usually, the continuum model is considered in the framework of the finite element method. The idea of the application of BEM in multi scale modelling was proposed in (Mrozek et al., 2006). In this approach, the material behaviour at the atomic level can be simulated and the total number of degrees of freedom is reduced, because in most cases only a small part of the multi scale model contains atoms and BEM does not need discretisation of

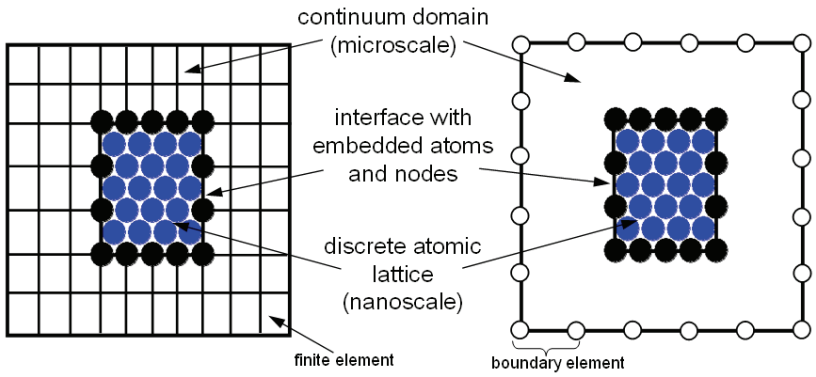


Fig. 6. The coupled continuum-atomic multi scale model.

the continuum's domain. The discrete scale is modelled using the Lennard-Jones potential, but for more realistic computations, more complex potentials such as the Embedded-Atom-Method (Daw & Basket, 1983) should be used. The presented multi scale algorithm can be used for different types of interatomic potentials. The potential parameters in the atomic scale can be obtained using results from *ab initio* computations (Mishin & Farkas, 1999).

The illustration of this multi scale model is shown in the Figure 6. The discrete atomic model occupies only a rather small area of the model, where the simulation at the nanoscale should be performed. The rest of the considered structure is modelled using FE or BEM, respectively.

The algorithm to solve the coupled multi scale model is presented in the Figure 7.

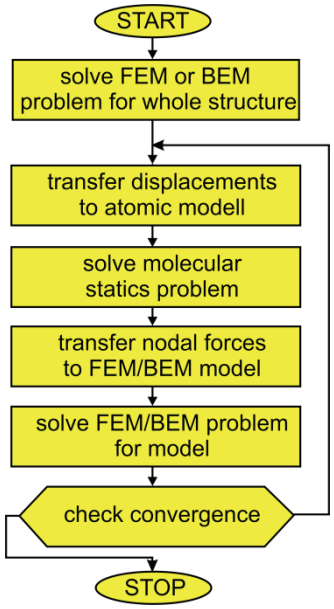


Fig. 7. The algorithm of solving coupled atomistic-FE/BEM model

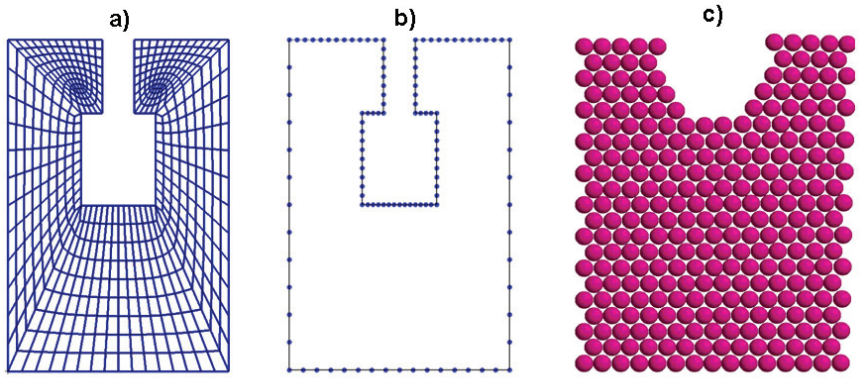


Fig. 9. a) FE mesh, b)BEM mesh, c) discrete atomic lattice

In the first step, the micro scale boundary conditions are applied and the continuum model is solved (Figure 7). Displacements of the interface atoms are obtained and introduced as initial displacements of the outer boundary of the atomic lattice. In the next step, the equilibrium positions of the atoms in the nano scale model are computed, using the method described in the previous section. Finally, forces acting on the interface atoms are computed and introduced as nodal forces to the continuum model. These computations are repeated iteratively until the stop condition is satisfied. The stop condition is executed when the difference between displacements of the embedded atoms during two iterations is less than an assumed admissible value.

3.2. Numerical examples

Some numerical examples are presented in the following section to illustrate this approach. For simulation of the material behaviour at the nano scale, rectangular plates with different shaped notches are considered.

The plate under shearing load is shown in the Figure 8. The centre of the notch is modelled as a discrete atomic lattice (Figures 9, 10). The benchmark was performed using both FE and BEM, coupled with a molecular model. The meshes are presented in the Figure 9a and 9b, respectively.

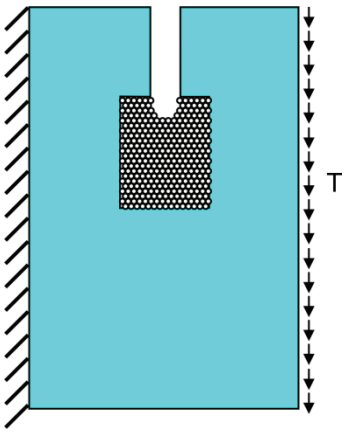


Fig. 8. Benchmark - plate with U-notch

The left side of the plate is constrained and the shear load is applied on the opposite side. Dimensions of the plate are 18x12 [nm^2]. The continuum model contains 61 quadratic elements and 244 degrees of freedom. The atomic model contains 282 aluminium atoms and 546 degrees of freedom. The Lennard-

Jones potential $\Phi(\boldsymbol{r}_{ij})$ was used:

$$\Phi(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \qquad (3)$$

with the following parameters: the collision diameter σ = 0.2575[nm], the dissociation energy ε = 0.1699[nN·nm], r_{ij} is the distance between atoms. These values are taken from Sunnyk et al. (2002). The potential describes a material with properties close to the aluminium.

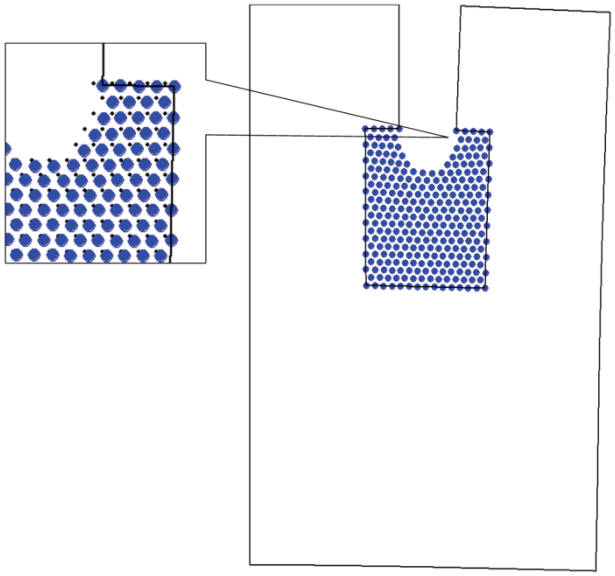


Fig. 10. Results of the simulation - equilibrium state under the shear load

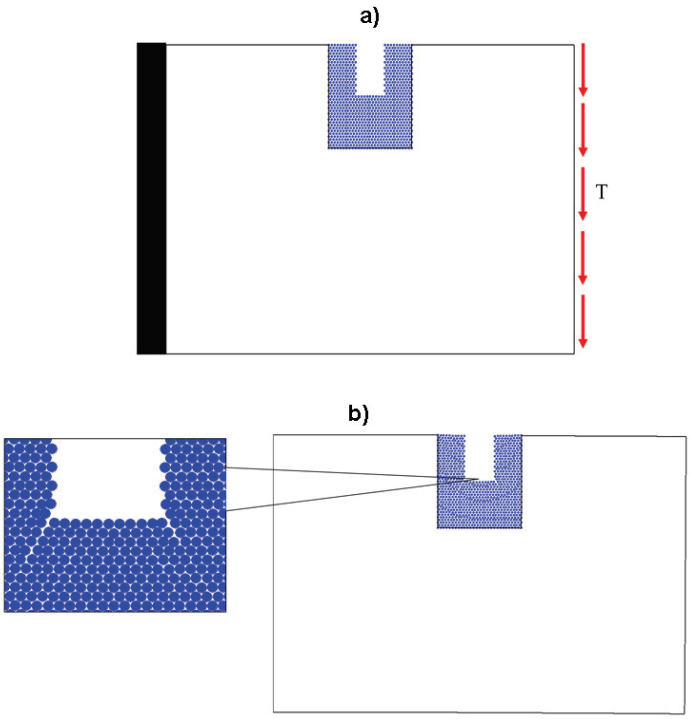


Fig. 11. The plate with U-notch under the shear load: a) initial equilibrium without load, b) equilibrium state under shear load

Table 1. Comparison of the convergence between BEM and FE coupled with discrete atomic model

Iteration	Maximal relative error at displacements %	
	BEM	FEM
1	302,5	352
2	82	3,2
3	51	0,6
4	3,4	0,01
5	1,6	0
6	0	-

Table 1 shows results of the numerical simulation and comparison of the convergence between BEM and FE. Faster convergence of FE arises from differences in discretisation of the domain and types of solvers used.

The next example is presented in the Figure 11. A plate with a rectangular notch under a shear load is considered. The entire left side of the plate is constrained and the shear load is applied on the right side. Dimensions of the plate are 40x27 [nm^2]. The boundary element method is applied to the continuum domain and consist of 113 quadratic elements. The atomic model contains 884 atoms (1768 degrees of freedom). The potential type and parameters are the same as before.

The results of the numerical simulations are presented in the Figure 11b. The atoms moved to find a new equilibrium state. Opening of the cracks at the corners (stress concentration areas) of the notch can be observed.

Another example is presented in the Figure 12. In this case, the bottom of the plate is constrained and the shear load is applied on upper boundary. The dimensions of the plate are 90x45 [nm^2]. Continuum model contains 176 quadratic elements. Atomic model contains 2033 atoms (4066 degrees of freedom). The parameters and material properties are the same as in the previous example.

Results of the numerical simulations are presented in the Figure 12b. Again, the opening of the crack at the centre of the notch can be observed. The middle layers of atoms moved in opposite directions and the new equilibrium state is achieved.

This kind of analysis provide the possibility to simulate, for example slips, crack behaviour and fracture at the atomic level.

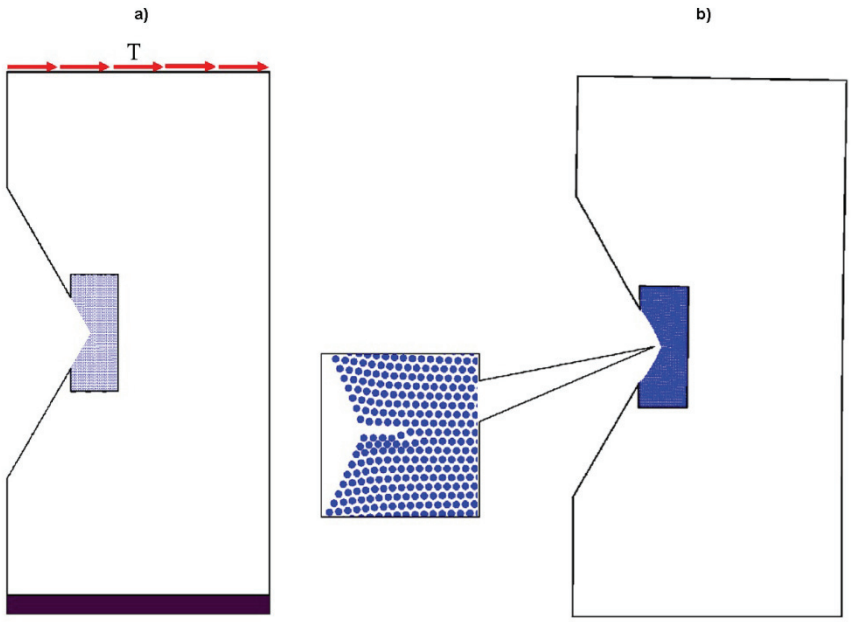


Fig. 12. Aluminium plate with V shaped notch under the shear load: a) initial equilibrium without load, b) equilibrium state under shear load

4. UPSCALING – CASE STUDY

As mentioned above, various continuum methods can be used to simulate macro behaviour of materials. The FE method is commonly applied to obtain complex description of the various phenomena described by the partial differential equations and this method is considered in all upscaling applications in the present work. FE is able to replicate real phenomena, which take place in the materials, as well as in the surroundings. In the present work the FE approach is used as the coarse scale method, which can be combined with the discrete methods (MC, CA, MD). A particular focus of this study is on the combination of FE and CA methods based on upscaling principles.

4.1. Multi Scale Cellular Automata – Finite Element (CAFE) Model for Strain Localization

The multi scale cellular automata – finite element (CAFE) model has been developed by the authors and applied to simulation strain localization for various forming processes. Details of the model can be found in earlier publications (Madej et al., 2006; 2007, 2007a). However the main principles of this method are repeated here.

According to the literature knowledge the micro shear band and shear band phenomena are the two processes taking place in the two different scales in the material. That is why two cellular automata spaces representing the material behavior in the micro- and mezo scale are introduced and are attached to the finite element code. This CAFE model is capable of simulation of the development of micro shear and shear bands at the micro and mezo scales respectively, eventually leading to strain localization in the macro scale. This approach is a typical example of the up scaling multi scale approach. A schematic illustration of the algorithm is presented in Figure 13.

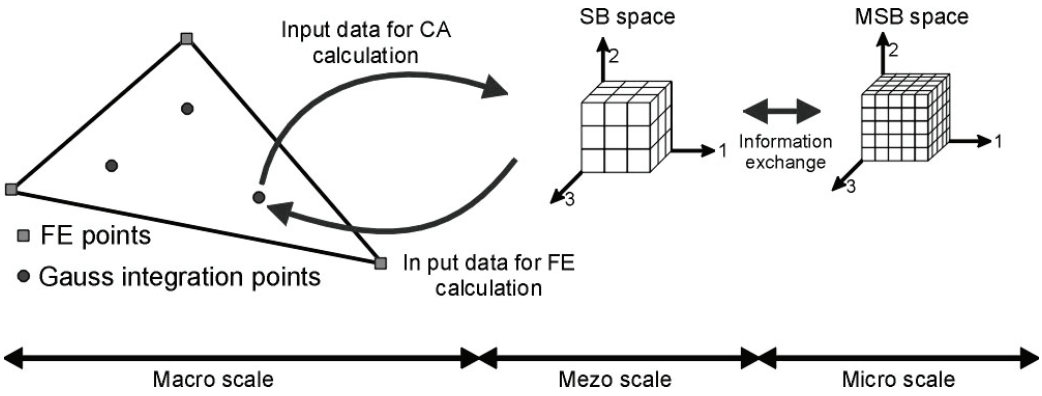


Fig. 13. Information flow between scales in the CAFE model for strain localization (Madej et al., 2007a)

In the CAFE model both CA spaces, micro shear band space (MSB space) and shear band space (SB space), are defined by several internal variables that describe each particular cell, as well as by a set of transition rules defined respectively for these spaces. The transition rules controlling changes between states in MSB and SB space are defined based on experimental knowledge (Korbel 1998, Cizek 2002).

Information about the occurrence of micro shear 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

macro scale to mezo scale and micro scale as well as from micro scale and mezo scale to macro scale. In each time increment, information about the stress tensor is sent from the finite element solver to the SB and than MSB space, where the development of micro shear bands is calculated according to the transition rules. After exchange of information between CA spaces, transition rules for the SB space are introduced, and propagation of the shear bands is modelled. Based on the information supplied by the CA spaces the correction coefficient ξ is calculated. This coefficient is sent to the FE program and used to modify the flow curve in the next step of FE calculations.

$$\sigma_p = \xi f(\varepsilon, \dot{\varepsilon}, T) \tag{4}$$

where: σ_p – equivalent stress, ξ – correction coefficient, ε – strain, $\dot{\varepsilon}$ – strain rate and T – temperature.

4.2. Examples of simulation.

The developed CAFE model is flexible and can be applied to simulation of common plastometric tests i.e. ring, uniaxial, plain strain compression as well as of any metal forming process, in which problems of the influence of micro shear and shear bands on crack resistance, final structure and properties of products are important. Selected examples of results obtained from conventional FE approach and the CAFE model for plastometric tests are presented in Figure 14-18.

The differences in material flow between cylinder compression and ring compression tests for aluminium are presented in Figures 14 and 15. Both samples are deformed up to a strain of 0.4 and the predicted strain distributions at the cross sections for a friction coefficient 0.12 are compared. Due to symmetry only a half of the samples cross section is presented in these figures.

Some strain localization during RC compression is seen in Figure 14 when the CAFE model is applied. This indicates that shear bands influence material flow during deformation, and may lead to a reduction in flow stress. The RC results are compared with the UC results presented in Figure 15. UC compression at strain 0.4 does not reveal any influence of shear bands on strain localization. Results obtained from the FE and CAFE models are comparable, and the material flow is homogenous.

Strain localization plays a significant role during plain strain compression. Examples of simulation of the plain strain compression of copper samples in channel die are presented in Figure 16.

As presented the CAFE model is capable of a more realistic material description than the FE approach, with a much clearer representation of the strain localization. Detailed discussion about the CAFE model capabilities in application to industrial problems is described in (Madej et al., 2007b, Madej et al., 2007c).

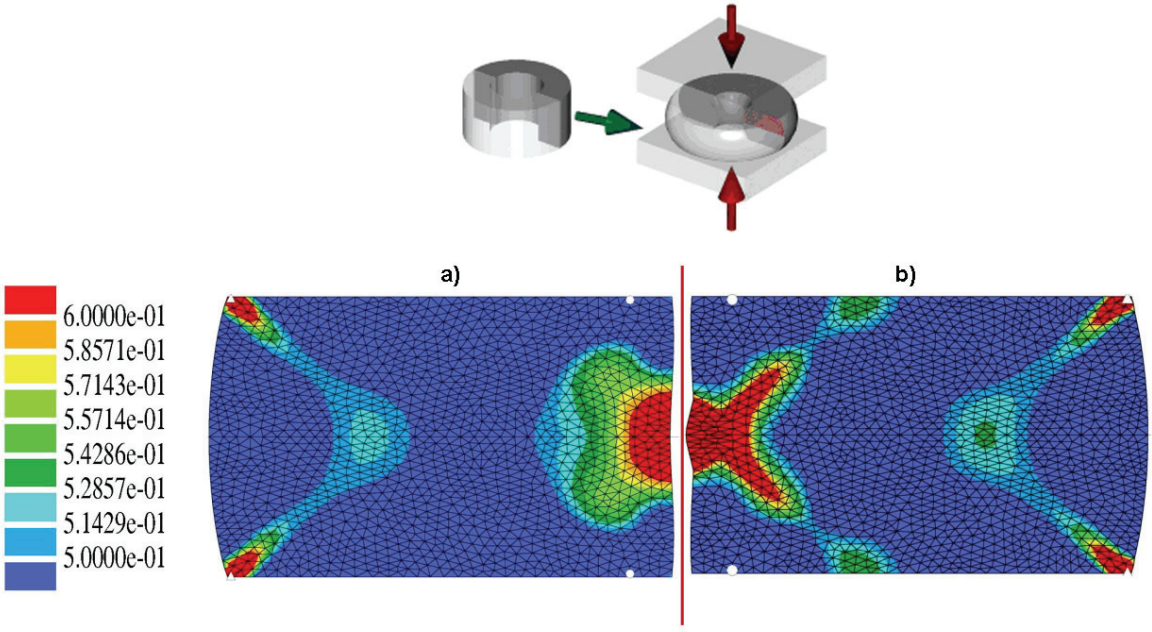


Fig. 14. Strain distribution at the RC test predicted by a) the FE with conventional constitutive law and b) the CAFE approach

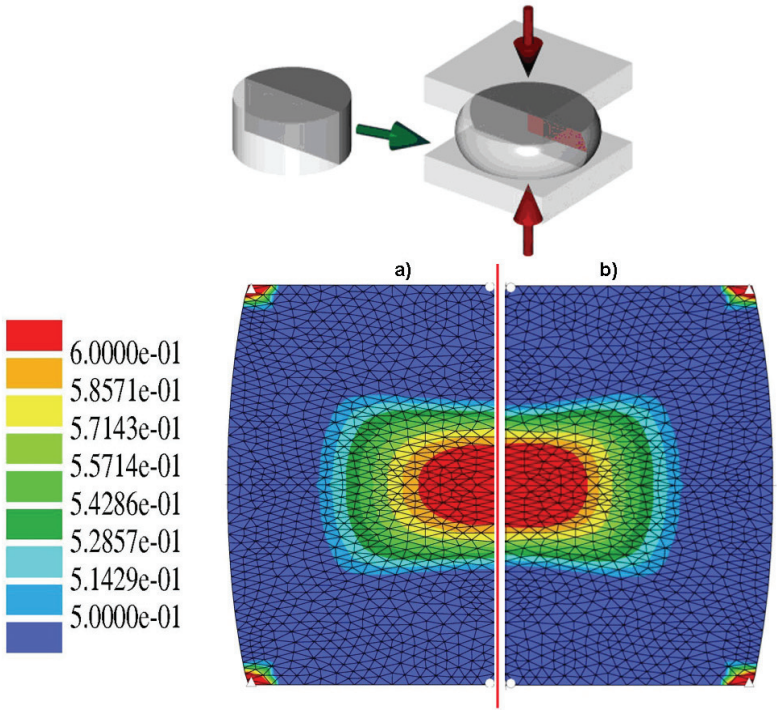


Fig. 15. Strain distribution at the UC test predicted by a) the FE with conventional constitutive law and b) the CAFE approach

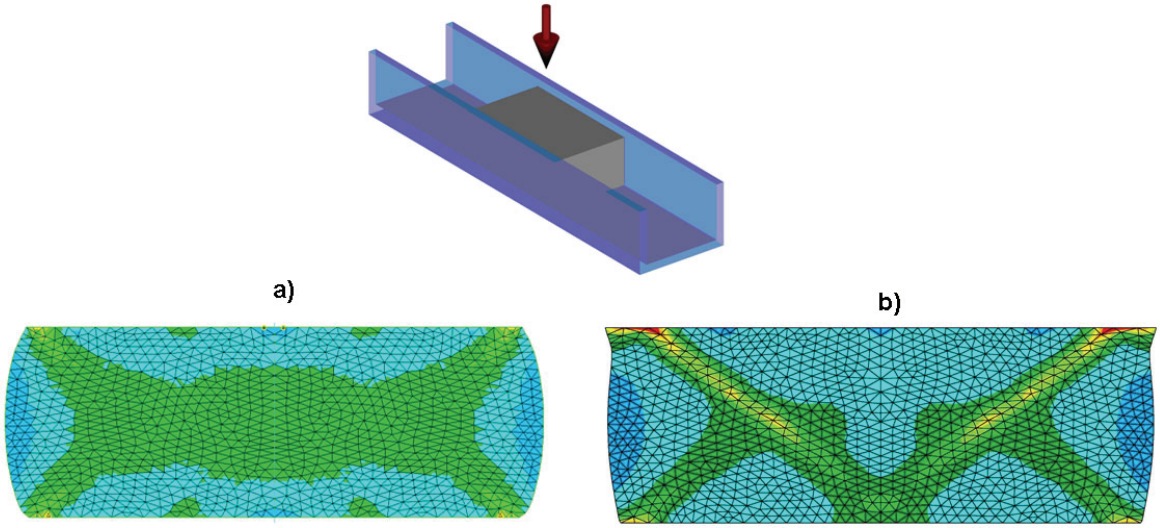


Fig. 16. Comparison of the strain distribution obtained in the channel die test from a) the FE and b) the CAFE approach

However the CAFE method is in principal a FE approach, and in some aspects is characterized by the same disadvantages i.e. mesh sensitivity. To investigate this behaviour a series of numerical simulations of the channel die compression (Figure 17) was performed with three different mesh densities: coarse, medium, fine.

It is seen in Figure 17 that the CAFE model is mesh sensitive. The largest values of strain are observed in Figure 17c for the fine mesh. However, despite these differences the shape of the localized zone is similar for all three cases.

During the numerical investigation the stochastic character of the CAFE model was revealed. As seen in Figure 18 strain localization bands can develop in two different directions, despite the same process conditions. This behaviour is in agreement with the experimental observations where families of shear bands develop in the same manner. This behaviour is not present for the conventional FE approaches.

During further work to obtain even more accurate results by the CAFE model the geometrical features such as grains, grain boundaries, inclusions etc. have to be included in an explicit way in the model and the new up scaling approaches have to be developed.

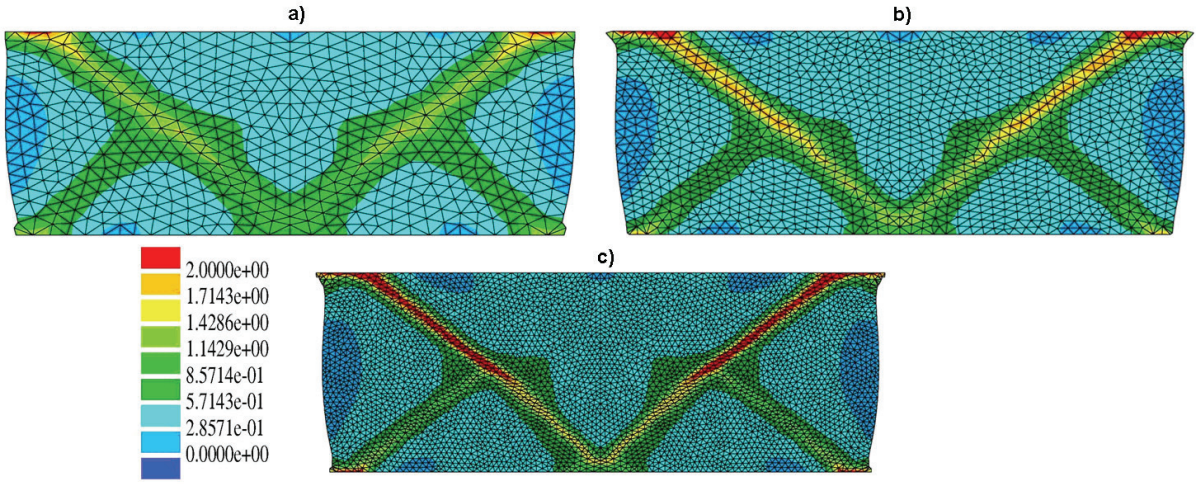


Fig. 17. Strain field obtained from the CAFE approach applied to simulate compression in channel die test for three FE mesh densities

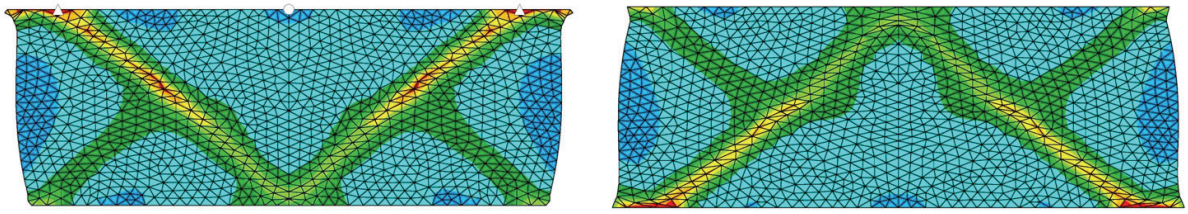


Fig. 18. Strain field obtained for the same process conditions from the CAFE approach revealing stochastic character of the model

5. CONCLUSIONS

Based on the presented literature survey it can be concluded that the number of multi scale methods and novel applications is growing significantly. There is a need to develop modern multi scale models in application to i.e. ingot melting, casting, welding, laser treatment, fusion welding**,** forging, friction stir welding, profile drawing, flow/spin forming, flat and shape rolling, ring rolling, stretch forming, deep drawing, semi-solid metalworking, plasma arc melting, highly filled material processing, injection moulding, blow or compression moulding, vapour deposition, molecular beam epitaxy, joining and several other. That is why there is a further need for classification of the available methods and systematisation of their applications.

The concurrent and upscaling multi scale approaches were discussed based on the two case studies: combination of the boundary and finite element methods with atomic model and cellular automata with finite element model, respectively. Examples of simulations as well as discussion of problems and difficulties related to these approaches were presented. Both models proved their capability to include in the solution stochastic and discontinuous phenomena taking place during deformation. This possibility to include stochastic phenomena which additionally take place at the same time in different scales in the material is the greatest advantage of the discrete methods (CA, MD, MC). This makes the developed multi scale models very powerful investigative tools in comparison to the conventional approaches.

Due to the advanced nature of described computational techniques there is a need for cooperative work between researchers handling the same problems during application of the multi scale methods.

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REFERENCES

Abraham, F.F., Broughton, J.Q., Berstine, N., Kaxiras, E., 1998, Spanning the continuum to quantum length scales in a dynamic simulations of brittle fracture, *Europhys. Lett.* 44, 783-787

Allix, O., 2006, Multiscale strategy for solving industrial problems, *Comp. Meth. Appl. Sci.*, 6, 107-126.

Belytscho, T., Lochnert, S., Song, J.-H., 2007, Multiscale aggregating discontinuities (MAD): A method for circumventing loss of stability, Int. J. Num. Meth. Eng., 69, (in press).

Burczynski, T., Mrozek, A. Kuś, W., 2007, A computational continuum-discrete model of materials, *Bulletin of the Polish Academy of Sciences,* 50, 1, 85-89

Burczynski, T., 1995, *The Boundary Element Method in Mechanics*, WNT, Warszawa.

Cizek, P., 2002, Characteristics of shear bands in an austenitic stainless steel during hot deformation, *Mat. Sci. Eng.* A324, 214-218.

Das, S., Palmiere, E.J., Howard, I.C., 2002, CAFE: a tool for modelling thermomechanical processes, *Proc. Conf. Thermomech. Processing: Mechanics, Microstructure & Control*, eds, Palmiere, E.J., Mahfouf, M., Pinna, C., Sheffield, 296-301.

Das, S., Abbod, M.F., Zhu, Q., Palmiere, E.J., Howard, I.C., Linkens, D.A., 2007, A combined neuro fuzzy-cellular automata based material model for finite element simulation of plane strain compression, *Comput. Mater. Sci*., (in press)

Daw, M.S., Basket, M.I., 1983, Semiempirical, quantum mechanical calculation of hydrogen embrittlement in metals, *Phys. Rev. Lett.* 50, 1285-1288

De Borst, R., 2007, Challenges in computational materials science, multiple scales, multi-physics and evolving discontinuities, *Computational Material Science*, (in press).

Demkowicz, L., Rachowicz, W., Devloo, P., 2002, A Fully Automatic hp-Adaptivity, *J. of Scientific Computing*, 17, 127–155.

Dumett, M. A., Vassilevski, P., Woodward, C.S., 2002, A multigrid method for nonlinear unstructured finite element elliptic equations, *SIAM J. on Scientific Computing*, 1-19.

Estrin, Y., 1996, Dislocation Density Related Constitutive Modelling, in: *unified constitutive laws of plastic deformation*, (eds), Krausz, A.S., Krausz, K., Academic Press.

Gandin, C. A., Rappaz, M., 1994, A coupled finite element - cellular automaton model for the prediction of dendritic grain structures in solidification processes, Acta Metall., 42, 2233–2246.

Gandin, C.A., Rappaz, M., 1996, 3D cellular automaton algorithm for the prediction of dendritic grain growth, Acta Metallurgica, 45, 2187-2195.

Gawąd, J., Pietrzyk, M., 2007, Application of cafe coupled model to description of microstructure development during dynamic recrystallization, *Archives of Metallurgy and Materials*, 52, 257-266.

Grosman, F., 1997, Application of the Flow Stress Function in Programmes for Computer Simulation of Plastic Working Processes, *J. Mat. Proc. Technol*., 64, 169-180.

Hirt, G., Kopp, R., Hofmann, O., Franzke, M., Barton, G., 2007, Implementing a high accuracy Multi-Mesh Method for incremental Bulk Metal Forming, *Ann. CIRP*, 56, 313-316.

Lan, Y.J., Li, D.Z., Li, Y.Y., 2004, Modeling austenite decomposition into ferrite at different cooling rate in low-carbon steel with cellular automaton method, *Acta Materialia*, 52, 1721-1729.

Lan, Y.J., Xiao, N.M., Li, D.Z., Li, Y.Y., 2005, Mesoscale simulation of deformed austenite decomposition into ferrite by coupling a cellular automaton method with a crystal plasticity finite element model, *Acta Materialia*, 53, 991-1003.

Lee, P.D., Chirazi, A., Atwood, R.C., Wand, W., 2004, Multi scale modeling of solidification microstructures, including microsegregation and microporosity, in an Al-Si-Cu alloy, *Mat. Sci. Eng. A*, A365, 57-65.

Khvastunkov M.S., Leggoe J.W., 2004, Adapting cellular automata to model failure in spatially heterogeneous ductile alloys, Scripta Mater. 51, 309–31

Korbel, A., 1998, Structural and mechanical aspects of homogeneous and non-homogeneous deformation in solids, *Courses and Lectures – No. 386*, Springer, 21-98.

Kumar, M., Sasikumar, R., Kesavan, Nair P., 1998, Competition between nucleation and early growth of ferrite from austenite-studies using cellular automaton simulation, *Acta Metallurgica*, 46, 6291-6303.

Kundu, S., Dutta, M., Ganguly, S., Chandra, S., 2004, Prediction of phase transformation and microstructure in steel using cellular automation technique, *Scripta Mater*., 50, 891-895.

Madej, Ł., Hodgson, P.D., Pietrzyk, M., 2006, Multi scale analysis of material behavior during deformation processes, in: *Foundation of Materials Design*, eds, Kurzydłowski, K.J., Major, B., Zięba, P., Publ. Research Signpost, Kerala, 17–46.

Madej, Ł., Hodgson, P.D., Pietrzyk, M., 2007, Multi-scale rheological model for discontinuous phenomena in materials under deformation conditions, *Computational Materials Science*, 38, 685-691.

Madej, Ł., Hodgson, P.D., Pietrzyk, M., 2007, Comparison of the strain distribution obtained from multi scale and conventional approaches to modelling extrusion, *Solid State Phenomena*, 129, 25-30.

Madej, Ł., Hodgson, P.D., Pietrzyk, M., 2007, The validation of a multiscale rheological model of discontinuous phenomena during metal rolling, *Computational Materials Science*, 41, 236-214.

Mieche, C., 2003, Computational micro-to-macro transitions for discretized micro-structures of heterogeneous materials at finite strains based on the minimization of averaged incremental energy, *Comp. Meth. Appl. Mech. Engrg*., 192, 559-591.

Milenin, A., Muskalski, Z., 2007, The FEM simulation of cementite lamellas deformation in pearlitic colony during drawing of high carbon steels, *Proc. Conf. Numiform 2007*, eds, Cesar de Sa, J.M.A., Santos, A,D., Porot, 1375-1380.

Mishin, Y., Farkas, D., 1999, Interatomic potentials for monoatomic metals from experimental data and *ab initio* calculations., *Physical Review*, 59, 5, 3393-3407

Missoum-Benziane, D., Ryckelynck, D., Chinesta, F., 2007, A new fully coupled two-scale modeling for mechanical problems involving microstructure: The95/5 technique, *Comp. Meth. Appl. Mech. Eng.*, 196, 2325-2337.

Mrozek, A., Kuś, W., Burczyński, T., 2006, Analisis of the Material Behaviour at the Nanoscale, *Proc. 35th Solid Mechanics Conference*, Kraków, 283-284.

Mrozek, A., Kuś, W., Burczyński, T., 2007, Application of the coupled boundary element method with atomic model in the static analysis, *Computer Methods in Materials Science*, 7, 284-288.

Nemat-Nasser, S., 1999, Averaging theorems in finite deformation plasticity, *Mech. Mater*. 31, 493-523.

Paszyński, M., Kurtz, J., Demkowicz, L., 2006, Parallel fully automatic hp-adaptive 2D finite element package, *Comp. Meth. Appl. Mech. Eng*.,195, 711-741.

Pietrzyk, M., 1990, Finite element based model of structure development in the hot rolling process, *Steel Research*, 61, 603-607.

Pietrzyk, M., Madej, Ł., Szeliga, D., Kuziak, R., Pidvysotskyy, V., Paul, H., Wajda, W., 2006, Rheological Models of Metallic Materials, *Research in Polish Metallurgy at the Beginning of XXI Century*, ed., Świątkowski, K., Komitet Metalurgii PAN, Kraków, 325-346.

Quested, T.E., Greer, A.L., 2005, Grain refinement of Al alloys: Micromechanisms determining as-cast grain size in directional solidification, *Acta Mater.*, 53, 4643-4653.

Rondanini, M., Barbato, A., Cavalloti, C., 2006, A multi scale model of the Si CVD process, *Proc. Conf., MMM, Freiburg*, 98-101.

Roucoules, C., Pietrzyk, M., Hodgson, P.D., 2003, Analysis of work hardening and recrystallization during the hot working of steel using a statistically based internal variable method, *Mat. Sci. Eng*., A339, 1-9.

Sfantos G.K., Alibadi M.H., Multi-scale boundary element modeling of material degradation and fracture, Computer methods in applied mechanics and engineering, 196, 2007, 1310-1329.

Shterenlikht, A, Howard, IC., 2006, The CAFE model of fracture - application to a TMCR steel, *J. Fatigue and Fracture of Engineering Materials and Structures*, 29, 770 – 787.

Sunyk, R., Steinmann, P, 2002, On higher gradients in continuum-atomistic modelling, *Int. J. of Solids and Structures* , 40, 6877-6896,

Szeliga, D., Gawąd, J., Pietrzyk, M., 2006, Inverse analysis for identification of rheological and friction models in metal forming, *Comp. Meth. Appl. Mech. Engrg*., 195, 6778-6798.

Tadmor, E.B., Oritz, M., Philips, R., 1996, Quasicontinuum analysis in crystals, *Phil. Mag.*, A 73, 1529-1563

Takatani, H., Gandin, Ch.A., Rappaz, M., 2000, EBSD characterization and modellling of columnar dendritic grains growing in the presence of fluid flow, *Acta Materialia*, 48, 675-688.

Thevoz, Ph., Gandin, Ch.A., 2001, Micro-macroscopic solidification models, *Encyclopedia of Materials: Science and Technology*, Elsevier, 5637-5642.

Vandyoussefi, M., Greer, A.L., 2002, Application of the cellular automata-finite element model to the grain refinement of directionally solidified 1l-4.15 wt% Mg alloys, Acta Mater., 50, 1693-1705.

Van Houte, P., Kanjarla, A.K., Val Bael, A., Seefeldt, M., Delannay, L., 2006, Multiscale modelling of the plastic anisotropy and deformation texture of polycrystaline materials, *Eur. J. Mech. A-solid.*, 25, 634-648.

Volker, J., Songul, K., Kaya, L., 2006, A two-level variational multiscale method for convection-dominated convection–diffusion equations, *Comp. Meth. Appl. Mech. Eng*., 195, 4594-4603.

Yang, X.L., Dong, H.B., Wang, W., Lee, P.D., 2004, Microscale simulation of stray grain formation in investment cast turbine blades, *Matl Sci. Eng. A*, A 386, 129-139.

Yazdipour, N., Davis, C.H.J., Hodgson P.D., 2007, Simulation of dynamic recrystalization using random grid cellular automata, *Computer Methods in Materials Science*, 7,168-174.

Yu, Q., Esche, S.K., 2005, A multi-scale approach for microstructure prediction in thermo-mechanical processing of metals, *J. Mater. Proc. Tech*., 169, 493–502.

Zhang, L., Zhang, C.B., Wang, Y.M., Wang, S.Q., Ye H.Q., 2003, A cellular automaton investigation of the transformation from austenite to ferrite during continuous cooling, *Acta Materialia*, 51, 5519-5527.

HYBRYDOWE I HIERARCHICZNE MODELE ANALIZY WIELOSKALOWEJ

Streszczenie

W pracy zaprezentowano dynamicznie rozwijające się nowe metody obliczeniowe do analizy wieloskalowej, umożliwiające opis zjawisk zachodzących w materiale, niemożliwych do przewidywania tradycyjnymi metodami modelowania. Dokonano klasyfikacji metod na dwie grupy różniące się sposobem podejścia do symulacji w różnych skalach oraz do interakcji między nimi. Pierwsza z nich to grupa metod hierarchicznych, która bazuje na reprezentatywnym elemencie objętości. Druga grupa to metody symulujące dane zjawisko w całej lub w części objętości badanego materiału równocześnie w kilku skalach. Przyjęto nazywać je metodami hybrydowymi odzwierciedlając współbieżne prowadzenie obliczeń różnymi metodami w przeciwieństwie do metod hierarchicznych, gdzie obliczenia prowadzone są w reprezentacyjnych elementach objętości. Opisano interesujące modele bazujące na połączeniu metod analizy mikro np. Automatów Komórkowych (ang. CA), Monte Carlo (ang. MC) czy Dynamiki Molekularnej (ang. MD) z metodami analizy makro np. Metodą Elementów Skończonych (ang. FE) czy też Metodą Elementów Brzegowych (ang. BE). Przykłady tworzenia i zastosowania modeli hierarchicznych i hybrydowych w zastosowaniu do symulacji zjawisk zachodzących w materiale podczas odkształcania przedstawiono bazując na połączeniu metod CA i FE oraz MD i BE.

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