Complex Modelling Platform based on Digital Material Representation

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Abstract. Proposition of innovative software platform dedicated to modelling of metallurgical processes is presented in the paper. Developed approach is based on the idea of material representation in the form of digital data sets describing various material properties in different length scales. The platform is equipped with additional software modules dedicated to support data gathering, microstructure image analysis, mesh generation and performance of multiscale simulations. The latter module, based on Cellular Automata – Finite Element (CAFE) method, contains two algorithms related to modelling of microstructural phenomena occuring in material during deformation under varying conditions i.e. micro shear and shear bands analysis and recrystallization modelling. The complex approach described in this paper allows not only knowledge based prediction of detailed material properties after thermomechanical metallurgical processes but it also gives possibility to modell entire life cycle of considered material. Thus, it facilitates the investigation of properties of final products and their development by strong quality improvement. Moreover, the platform allows to limit costs of manufacturing by reduction of many expensive industrial trials and their replacement by pure virtual research. Some of the results obtained from application of selected software modules are presented in the paper.

Keywords. Digital material, multiscale modelling, microstructure image analysis.

1 Introduction

Numerical modelling is currently applied to predict material behaviour under manufacturing and exploitation conditions. The most commonly used method for this purposes is Finite Element Method (FEM), which can be applied to simulate a variety of problems, from simple experimental tests (e.g. tensile, torsion) to sophisticated processes consisted of complex structures and systems (e.g. cars, building, implants). FEM is able to simulate real processes occuring inside the material and its environment (tools), as well as interactions between them. Althought the method is becoming introduced in industrial aplications, it still

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requires development to improve the results of performed simulations. Thus, in recent years many modifications of FEM methods were develped e.g. *hp*-adaptation, non-continuous finite elements, etc. [1]. Nevertheless, there still exists a lot of constraints. Some of them are related to possibility of prediction the microstructural phenomena, which proceed simultanously in different length scales.

Another constraints are related to FEM high computational complexity, while the industrial companies expect short time of calculations. Therefore, alternative modelling methods are being developed [2]. The main objective of such techniques is focused on improvement of their efficiency and enhancement of the quality of obtained results, including material behaviour in all length scales. The models equipped with such methods facilitate designing of new materials and analysis of their behaviour during processes, which proceed on manufacturing and exploitation stages of materials' life-cycle. The papers published recently contain the propositions of innovative multiscale models, which take into consideration sophisticated material behaviour including microstructural phenomena. One of such approaches is Digital Material Representation (DMR), which offers the possibility of modelling in various length and time scales [3, 4]. The methodology can be used in models based on FEM as well as other alternative techniques like cellular automata (CA).

Contribution to development of the complex modelling platform based on DRM is the objective of this work. The review of the solutions available in the DMR field is presented in the subsequent section. Section 3 contains design and implementation details of proposed modelling platform, which is closely related to the idea of DMR but also equipped with additional simulation modules. The results generated by this platform are presented and discussed in section, 3 as well.

2 Idea of Digital Material Representation

The DMR offers possibility of material description in a complex form, which consists of various sets of metalurgical data. These components gather and analyse information that characterize material structure and properties in various scales. Thus, the input data for computer modelling methods, e.g. FEM or CA, can be easily prepared on the basis of such representation.

The more precise DMR is applied, the more realistic results of calclulations regarding material behaviour are obtained. Due to that solution, the detailed virtual analysis of simulation results can be performed, while errors of calculations are minimized. This allows the replacement of conventional methods, dedicated to determination of material properties, by the computer automatic analysis, which connects DMR with manufacturing processes modelling and with digital analysis of results (Figure 1).

The DMR concept was created quite recently, therefore, there are only few scientific publications, which consider this methodology. Interested approaches based on the idea of DMR are presented in [3, 4]. The basic assumptions of the proposed system in [3] joins the material structure with its basic properties, including grains morphology and texture. Such synthesized material is deformed and then investigated to obtain the properties of product after processing. The required additional data, like material phases, grains rheological models or their chemical composition, are stored in the external database. Since in this approach the phenomena occurring in other scales are not taken into consideration, the final results are reliable mainly in the macro scale analysis.

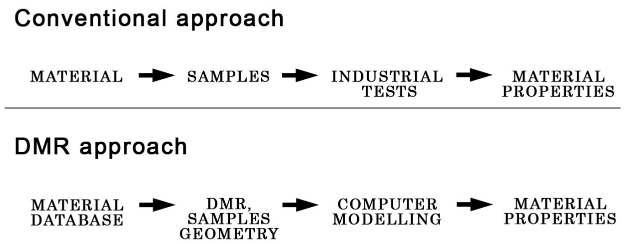

Figure 1. DMR basic concept in comparison to conventional approach [3].

The proposition presented in [4] is DIGIMICRO software, which supports 3D calculations based on DMR concept. The spatial microstructure is prepared by the Voronoi tessellation combined with additional optimization algorithms. The prepared material described by selected properties is used in simulations of compression tests. Simulations are performed using FE method, which is preceded by the process of microstructure anisotropic meshing. Final interpretation of results is facilitated by visualization module, which allows presentation of microsections sliced through the sample. Thus, the properties of digital material can be determined almost automatically and that reduces costs of real industrial trials. Works [3,4] became an inspiration for the Authors of this project to develop multiscale DMR engine, which is described below.

3 Multiscale DMR engine

The idea of computer system based on DMR methodology, which would be able to cope with problems of microstructural phenomena modelling in various scales and with analysis of real microstructures photographs, is presented in this work. The modelling platform equipped with such algorithms and external interfaces that are opened for new additional modules can be treated as a complex modular approach to modelling material behavior.

The main idea of the proposed modelling platform is presented on the first level deployment diagram in Figure 2. The basic DMR engine placed in the center of this scheme is responsible for interactions with users as well as for dynamic analysis and exchange of data between proposed modules. The subsequent steps of DMR engine algorithm can be enumerated as follows:

- Input data– it contains required initial conditions of the experiment gathered from users e.g. type of material, photograph of its microstructure, geometry of samples, type of experiment, range of temperatures, forces, etc.

- Reasoning – accordingly to the values of input parameters, the proper modules are selected e.g. dynamic recrystallization can be applied dependently on the range of temperatures and type of material
- Modelling – this stage consists of material structure preparation and its proper description, which is sent as DMR data. Afterwards the selected modelling algorithm is applied
- Visualization and interpretation – the last step is responsible for presentation of obtained results in the form of various 2D plots.

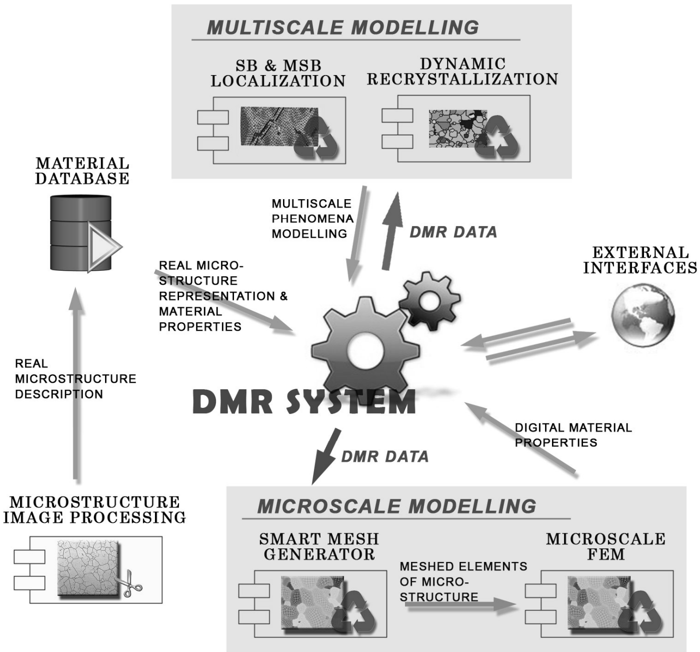

Figure 2. Main idea of developed complex modelling platform.

Each module presented in Figure 2 was designed and implemented (most of them in C++ and C#) by the Authors. Detailed specifications of particular modules functionality are presented in the following subsections.

3.1 Database Engine and Image Processing Support

The proposed database is implemented in relational database management engine MySQL and consists of five groups of tables. The first is dedicated to gathering of material properties, which describe specific material parameters in terms of environment termperatures and related metallurgical processes. Another tables store chemical composition of material and its rheological features. The next group is dedicated to general information, e.g. names or categories of materials. The last one gathers information about users, their passwords and contact data. The material database was implemented and is still developed as an internal project of MiTI

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Additionally, the module supporting data acquisition is attached to the system. The main objective of proposed module is processing of real microstructure photographs, gathered from optical microscope, and their automatic analysis to obtained digital representation of material microstructure [5]. The module's functionality is based on the usage of two internal algorithms i.e. modified Canny Detector [6] and Dynamic Particles filtering method [7]. The final result is presented in form of coloured image of microstructure, where each grain is marked with different colour. Moreover two text files containing grain borders description for meshing purposes and statistical characteristics of material are generated.

Presented above idea of the digital material representation directly fulfil the increasing need for accurate input data for advanced numerical analysis of material behaviour under loading conditions. Macroscopic material response is a result of complex interactions of various phenomena taking place in material at the same time but in different scales. Commonly used numerical approaches describe material behaviour mainly in macro scale. However, works related to nano or micro scale simulations using FE are becoming more and more popular [8].

3.2 Microscale Modelling

The meshing process consists of two tasks: (a) preparation of a special *control space* structure to provide the required sizing of elements throughout the domain and (b) discretization of the domain following the control space as closely as possible. The sizing information in the control space is stored in the form of an anisotropic metric and it can be automatically gathered from two geometrical sources, either from the user input or from the numerical adaptation process. All available sources are processed and stored in a single adapted control space (either quadtree or background mesh) structure using an adaptive procedure [9]. In the presented approach the control space is initialized with a uniform coarse sizing, which can be then further refined in a convenient way, by introducing a number of discrete metric sources at the areas of interests. After all discrete sources are inserted, the metric field is adjusted according to the prescribed element size gradation and it is then used for guiding the generation of a triangular mesh.

The meshing procedure starts with the discretization of domain contours. The created boundary points are triangulated using a modification of the Delaunay incremental insertion algorithm working in Riemannian space. The constrained triangulation is obtained by recovering all missing edges and removing obsolete elements. A number of additional points are inserted within the domain in order to achieve a *unit mesh* (i.e. mesh, where all edges have unitary metric length) property according to the control space. If the quadrilateral mesh is requested, a conversion procedure can be used. Finally, several methods of mesh post-processing are applied in order to improve the quality of elements (Figure 3).

Prepared mesh on the basis of the DMR can be used during investigation of behaviour of particular grains with different properties i.e. different crystallographic orientation.

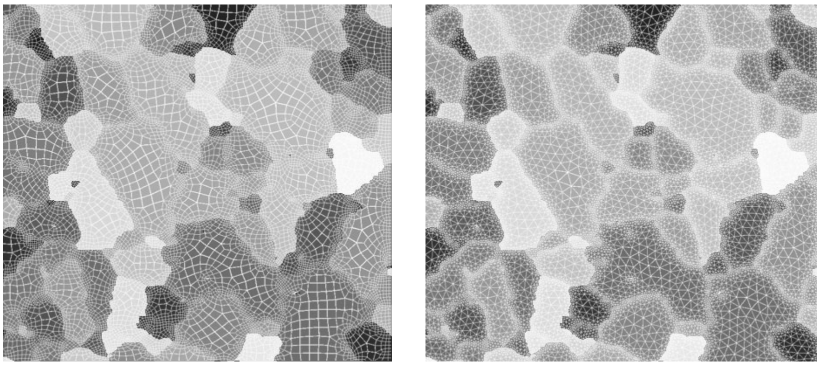

Figure 3. Digital microstructure obtained from the optical microscope image with applied mesh on the grains area.

Analysis of phenomena, which occur in the scale of single grains and their interactions, is a key to solve various problems that modelling of deformation processes has to face, i.e. the change in the deformation path, strain localization. Since such an analysis is crucial to support experimental observations, scientists are trying to capture these microscale processes [10].

3.3 Multiscale Phenomena Simulation

Disadvantage of conventional modelling techniques is lack of possibility to include discontinuous nature of material behaviour. A hybrid method based on the combination of Cellular Automata and Finite Element technique [11] overcomes that limitation and is one of the alternative numerical solutions. CA method is usually used to described material behaviour in micro and mezo scale. This method found wide range of application in simulation of microstructural changes i.e. modelling of static and dynamic recrystalization [12, 13]. The initial microstructure, with its geometry explicitly represented in the cellular automata space, is one of the key parameters that influence accuracy of the final results in these applications. DMR method provides a complex tool for such input data preparation (grain size, shape or grain orientation, material properties, etc.) used during further CA or CAFE calculation of micorstructure changes e.g. dynamic recrystalization [12].

A multiscale CAFE modelling of strain localization phenomena is another field of DMR application. Authors of this work have developed a model capable of simulation the development of micro shear and shear bands in micro and mezo scale, respectively, eventually leading to strain localization in macro scale. Detailed description of the CAFE model is described elsewhere [14], and schematic illustration of the algorithm is presented in Figure 4.

In each time step, information about the stress tensor is sent from the FE solver to the MSB space, where the development of microshear bands is calculated according to the transition rules [14]. After exchange of information between CA spaces, transition rules for the SB space are introduced, propagation of the shear bands is modeled and modified stress value is than sent back to the FE code.

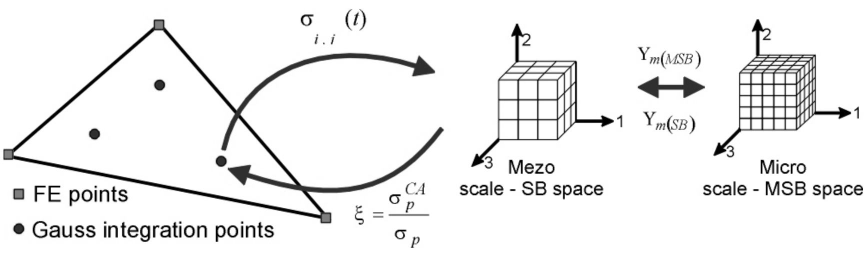

Figure 4. Information flow between scales in the CAFE model [14].

Comparison between results obtained from conventional FE approach and developed CAFE model is presented in Figure 5. It is seen in this figure that the CAFE model is capable to describe material behaviour more realisticly than the FE approach. However to obtain even more accurate results by the CAFE model the geometrical features such as grains have to be included in an explicit way in the model.

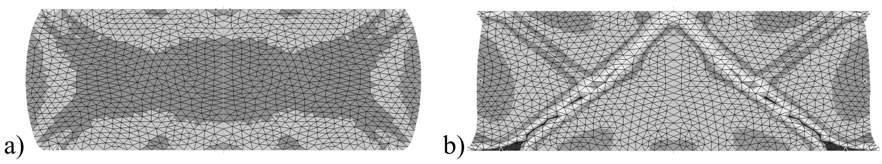

Figure 5. Strain distribution obtained from the a) FE and b) CAFE simulation.

At this stage of the CAFE model development the microstructure is considered in an implicit way. However, it is known from literature [10] that influence of grain shape, size or orientation on micro shear and shear band development is crucial. That is why during further work, presented idea of DMR will be added to the developed CAFE model and complex analysis tool will be established.

4 Conclusions

Following the concept of Digital Material Representation presented in [3, 4] the complex solution dedicated to investigation of material behaviour under loading condition in micro, mezo and macro scale was developed. Presented model is an example of multi disciplinary approach to material science. From one side image processing techniques and MySQL database system, from the other side mesh generation algorithms and multi scale computational methods. Such an approach gives opportunity to overcome difficulties in precise modelling of material behaviour in various scales, what is of importance from the industrial application point of view. Future work will focus on further development of the system to extend its capabilities and to cerate a user friendly environment.

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5 References

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