# RULE-BASED EXPERT SYSTEM APPLICATION TO OPTIMIZING OF MULTISCALE MODEL OF HOT FORGING AND HEAT TREATMENT OF TI-6AL-4V

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## 1 INTRODUCTION

Nowadays, multiscale methods are increasingly used in modeling of processes and designing of materials. However, there are two serious obstacles to wider application of such methods. One is a demand of computing power, which is present in almost all applications. Increasing of available computing power is not a solution. Exponential growth of computational complexity with increase of accuracy will always lead exceeding of available resources. Therefore, adaptation of multiscale models is important point of interest. The second obstacle is a difficultness of multiscale model design. Model is an abstraction of reality. Therefore, some assumptions have to be done – which phenomena are important and which do not. There is an additional point of interest in multiscale modeling – in which scale the particular phenomena can be modeled with a good balance of accuracy and computing power demand. Usually, there is no single good answer. Designing of a model can be seen as a kind of an optimization process, where the goal is a function of efficiency and reliability. The need of a such process is pointed out in many publications (e. g. [1]), but in the most of cases it have to be done by a researcher himself.

### 1.1 Adaptation of multiscale models

The term "adaptation" in computer science refers to a process, in which an interactive system (an adaptive system) adapts its behavior to individual users (use cases) basing on information acquired about its user(s) and its environment. In numerical modeling, an adaptation refers to modifying of model properties to improve its quality. Usually, numerical error or its estimation is assumed to be a criterion of an adaptation. However, the question is how to estimate error in a multiscale manner. There are many error indicators for single scale

models (e.g. [2] and many others). In a multiscale analysis, there are three main families of error indicators [3]. They are: multiscale reduction error estimators/indicators introduced by Fish and coworkers [4], localized modeling error estimates developed in the context of goal-oriented adaptive modeling by Oden and coworkers (e.g. [5]) and physically based error indicators introduced by Gosh and coworkers [6]. The first two families are based on an a'posteriori error estimator. The disadvantage of those methods is that a mathematical description of micro and macro scales phenomena must be consistent. Moreover, its application in regions with high gradients is difficult or even not possible. The physically based indicators are more flexible and can use various criteria. However, also in this case it is assumed, that error estimation can be directly computed.

For all of mentioned methods, a mathematical description of models in different scales must be known and analytically transformed before computational codes would be developed. It makes them not applicable if a more generous behavior is expected. Moreover they are not applicable when error estimation cannot be computed with mathematical equations or numerical procedures. This happens in two cases. First, a microscale model can be not compatible with a macroscale one in mathematical sense, than it will not be possible to project an error. FEM and Cellular Automata (CA) based models could be an example. Such models are quite common in modeling of a phase transformation [7], an microstructure evolution [8], thixoforming [9] and many others. There are no error estimators for CA simulations, furthermore there are no methods of projecting of error between FEM and CA. In the second case, phenomena which occur in a real material are not taking into account during modeling. While the numerical error can be very small, an absolute error, understood as a difference between a simulated and a real value can be extremely large.

### 1.2 Prediction of possible phenomena

Typical multiscale models consist of two models in two different scales, together with up- and downscaling (*projection*) procedures. Such models are able to predict usually only one microscale phenomenon, like a cracking, microscale heterogeneity or a microstructure evolution in well-defined conditions. An adaptation of such models could lead to results, which are very accurate from the numerical point of view, but completely different from a real material behavior. This happens, when a mathematical or a numerical description is not appropriate (the same as for example use of Galerkin method to a convection dominated problem in a single scale modeling), but also when the researcher did not take into account all possible phenomena. It enforces close cooperation of a numerical modeling and material science experts. Nevertheless, neglecting of important phenomena is still one of main reasons of modeling failures. On the other hand it is obviously not possible to take into account all possible phenomena. Nowadays, a prediction of possible phenomena and its significance must be done by researchers themself.

Reassuming: (a) classical multiscale models are applicable only in well-defined conditions, (b) existing multiscale error indicators are not able to predict the difference between a numerical solution and a real behavior and (c) it is expected to simplify the use of multiscale models. In this paper, a concept of an adaptation of a multiscale model with a rule-based

expert system is presented. With this methodology, the coupling between a multiscale models design and modeled phenomenological models is weakened. Moreover, capturing of phenomena which are not numerically modeled is feasible.

### 1.3 Knowledge Based Systems in numerical modeling

Knowledge Based Systems (*KBSs*) are widely used in a technologies design, but in the most of applications they are used instead of a numerical modeling, not for supporting it. KBS and a numerical model can cooperate in two ways: a numerical model can be a source of knowledge for KBS or KBS can be used for aiding of a numerical model development and controlling. Rec et al. [10] shown possibilities of a coupling of a rule-based system Rebit with a Finite Element Method (FEM) simulation of a rod rolling. In this paper, Rebit controls execution of FEM simulations, running computations and utilizing computations results in an inference process.

KBSs are also used to aid of a models development. Applications of KBSs to support of a finite mesh generation are relatively numerous. Sangiovanni [11] shown fuzzy logic rules used for a Finite Mesh design. Dolšak [12] presented the Prolog based FEMDES expert system, also for a finite mesh generation. Abd El-Ghany and Farag [13] presented an expert system that provides an intelligent interface between a testing engineer and a FEM software. Pinfold and Chapman [14] described DART system, aiding a FEM analysis design of automotive body structures with a KBS. Li and Qiao [15] shown a hybrid expert system for a FEM simulation of fuselage frame of an aircraft structure, which integrates an expert system with neural networks. Bellenger et al. [16] presented the framework for balancing between costs and quality of FEM analysis. They pointed out, that in industrial context not only accuracy, but also time of computations is crucial. Leitold et al. [17] and Németh et al. [18] described a problem of a models simplification. They did not use a KBS, but shown algorithm is in fact a set of rules for an expert system. It should be noticed, that almost all papers cited above refer to FEM. What is meaningful, there are no papers describing KBSs application in a multiscale modeling.

## 2 RULE-BASED MULTISCALE MODELLING

### 2.1 Agile Multiscale Modeling Method (AM3)

The most of presently developed multiscale models are designed as ”single author-single use” codes. It causes wasting of work, when the same problems are repeatable solved by different researchers. Also maintaining and improving of existing models are difficult. One of the possible solutions is designing of a unified multiscale modeling framework. The authors developed such a framework, combining a possibility of KBS based adaptation with a unification of communication between single scale models.

Due to generalization of communication interfaces, it is not possible to merge models in different scales basing on mathematical transformations. Still, material properties can be calculated with microscale results (upscaling) and initial/boundary conditions for microscale models can be calculated with macroscale models (downscaling).

AM3 based multiscale model architecture consist of a hierarchy of models in many (minimum 2, maximum *n*) scales. The minimal configuration is one coarse scale and two fine scale models. It is assumed, that a "*fine scale model*" is any computational or mathematical model, able to calculate material properties with given initial and boundary conditions. Those properties could be e.g. viscosity or a stress-strain curve.

Respectively, a "*coarse scale model*" is assumed to be a model, which needs material properties from an external fine scale model. It is important, that the coarse scale model does not communicate with the fine scale model directly, but via so called *Adapter*. The Adapter communicates with a KBS, in turn. A KBS decides, basing on supplied information, which fine scale model should be used to calculate material properties. The Adapter stores at least two, alternative fine scale models. They are able to calculate the same properties, taking into account different phenomena, with different accuracy and different computation power demands. From the coarse scale model point of view, it makes no difference which fine scale model had been used.

Fine scale models could be a self-sufficient one. It means that all properties, needed for calculations are known and dependent only on initial and boundary conditions. However a fine scale model can expect providing some properties from outside. In such case, a model is concurrently a fine and a coarse scale model (with different reference points). Due to such a structure it is possible to create a hierarchy of models. Its depth is limited only by computer power demand. Simultaneously, models do not have any knowledge about a hierarchy, they know only their own upscale and downscale interfaces.

A fine scale model could be a primitive (e.g. Newtonian viscosity), a mathematical formula (a function of one or more variables), a simple numerical model (e.g. an interpolation of tabularized data) or more complex numerical model (CA, FEM, Molecular Dynamic, etc.).

The core of this process is a KBS. It decide, which fine scale model should be used. A KBS can access all data from a coarse scale model and previous results from fine scale models. Knowledge, stored in a KBS should apply to two issues families, which are a justification of using of the particular fine scale model and estimated computational costs of it. It has to be remembered that more detailed models have more computing power demands. During reasoning, a fine scale model's reference is found. It is given to Adapter, who "transparently" manages a connection between fine and coarse scale models.

### 2.2 KBS

There are two main decisions to make during model setting-up. First, which phenomena should be modeled in particular scales? It is obvious, that increase of the number of phenomena taken into account rapidly increase computational complexity. On the other hand, neglecting of important behavior can make model useless. Second, location of fine scale models (in spatial and temporal sense) have to be chosen. Nowadays, defining of modeled phenomena is done by designer, basing on his knowledge of process and material behavior. Microscale models positioning is also done by designer, partially supported by automatic adaptation methods. Increase of the number of modeled phenomena has to be limited due to an available computing power.

Pattern of design is determined by previously chosen strategy of multiscale modeling. Methods which are described in literature are based on two solutions. In the first one, computations are performed on coarse model, then results are analyzed, and eventually computations are repeated by means of fine model. Such solution requires a great amount of time and provides no opportunity to predict final time of calculations. In the remaining solution, model designer tries to predict correct multiscale simulation's configuration. Usually it leads to acceptable, but far from optimal solution and requires highly skilled designers.

One of possible ways to improve quality of multiscale models is employing of Knowledge-Based Systems (KBS). KBS can be used as an alternative to precomputations, which are usually very resources consuming.

### 2.3 Rebit – Knowledge Based reasoning system

Rule-based system Rebit was developed at Management Faculty of AGH University of Science and Technology. From the point of view of functional approach, the basic task of the system is conducting the conclusion process upon the knowledge base chosen by the user. This task is executed by the rules engine in cooperation with the Rebit Client, which can be a human interface or other computer program. Knowledge representation language used in Rebit solution is enough expressive, as well as fully decidability. It allows writing in user-friendly form knowledge of material engineers. Likewise, correctness of knowledge in semantic point of view is possible. Due to application of SOA (service-oriented architecture), Rebit could be easily adapted to cooperate with multiscale modeling software.

An important feature of Rebit, allowing it to be used in multiscale modeling, is the possibility of suspending and resuming the process of inference at any time. It is possible to interrupt this process while saving the current state. In any moment, it is possible to resume the inference process, without any influence on a process. It gives an opportunity to acquire new knowledge when relevant information is not available in databases and starting the process from the beginning is impossible or not recommended. It is particularly important in case of multiscale simulation. Numerical models usually need long time to be solved. Thanks to suspending of inference process, the same engine can be used for other process or even turned off, if numerical computations are expected to take long time to finish. This ability could be used in parallelization of multiscale model. It is also useful in design time when some premises have to be obtained through in-depth studies.

Another important feature of Rebit System is its architecture. It is a service oriented system. The inference engine works as a web service according to Simple Object Access Protocol (SOAP) specification. This service can be consumed by SOAP clients running on any operating system. Rebit System is equipped with two generic clients, i.e. *desktop client* (in MS windows environment) and *thin client* (in any web browser). "Generic" in this case means the ability to manage the inference process on any Knowledge Base (KB) selected by the user. For AM3 based simulations, dedicated clients can be developed working with pre-defined KB in automatic way. One of advantages of dedicated clients is the possibility of extending a standard rule-based functionality. At the integration stage some workflow capabilities and additional flow controls or translations can be introduced.

Rebit System can be deployed as a fully distributed system, where each component resides on a different node. More integrated option, where engine, client and KBs repository are available as a completely autonomous application, is also possible.

The inference process in Rebit System (in both deployment scenarios) proceeds according to the following scheme. In the first step client has to obtain a KB. Next step depends on the type of inference process. In forward chaining mode a set of input variables has to be chosen and assigned. In backward chaining it is to formulate a hypothesis. Last type of inference, i.e. mixed inference, requires choosing one variable, called final, from the entire set of variables. At this point the inference engine starts interacting with the user (AM3 framework in this case). The aim of this stage is obtaining values for all variables needed to finish the inference process. As it was mentioned above, this stage can be suspended for an indefinite time and resumed afterwards. In the case of forward chaining the inference process ends up after firing all possible rules with input variable in their premises. Backward chaining is finished when we are able to reject or accept the hypothesis. The inference process in mixed mode ends up when it finds a value for final variable.

## 3 THERMO-MECHANICAL TREATMENT OF TI-6AL-4V

Components of the titanium alloy Ti-6Al-4V are often produced using hot forming processes. During those processes the influence of processing parameters on microstructure evolution is of high importance due to the effect on the final mechanical properties. In general the thermo-mechanical treatment is divided into several processing steps which are heating and soaking of the raw material on forming temperature, the forming process itself as well as the heat treatment afterwards.

The success of thermo-mechanical treatment relies on the control of microstructure evolution. Two of the most important microstructural mechanisms in hot processing of titanium alloys are grain coarsening and phase transformation. Mechanisms of phase transformation occur during heating and cooling whereas the effect of grain coarsening is dominant during soaking on forming temperature.

In addition during forming at high strain rates the adiabatic heating has to be taken into account due to its impact on microstructure. Those temperature changes caused by fast deformation can lead to a significant change in phase amounts and grain morphology [19].

## 4 NUMERICAL MODELLING

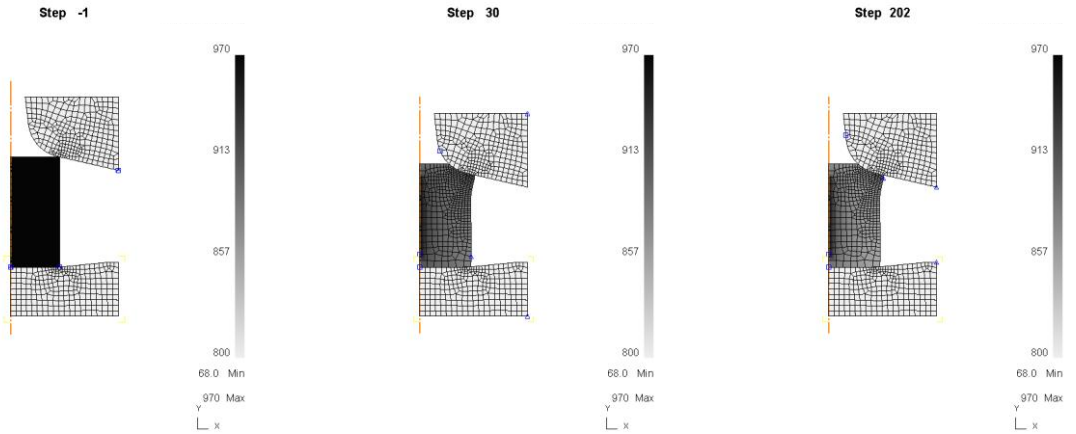
### 4.1 Macroscale model

The 2D simulation of thermo-mechanical treatment of forged components is done using the finite element (FE) software DEFORM2D$^{TM}$. For simulation of metal forming input data like material flow curves, friction coefficients as well as thermo-physical parameters, are required. In general those input data are verified by experiments. In the preparation of FE-simulation process parameters have to be defined were the forming temperature is of high importance beside die speed and stroke.

After simulation the results are shown in the form of strain and temperature distributions

for the simulated work piece. In addition the curves for temperature, strain and strain rate for every time step in each element are available. Those data are used as input for further modeling of microstructure evolution.

In this work, a simple process with an axisymmetric hot deformation of a billet has been modeled. The temperature on the axis of symmetry is given as a boundary condition, as well as the heat exchange with environment on outer surfaces of the billet. Between 200 and 220 seconds, the billet is deformed (Figure 1).




(a) (b) (c)

**Figure 1**: Temperatures [°C] and shapes of the billet on the beginning (a), after deformation (b) and at the end of the process (c).

### 4.2 Cellular Automata model

For a microstructure modeling of Ti-6Al-4V during a thermo-mechanical treatment the 2D Cellular Automata model (CA) had been created [8]. The CA model is based on a probabilistic approach which is capable to describe the grain coarsening behavior. To describe the microstructure the CA-model is using square shaped cells with different cell states. Furthermore, Moore´s neighborhood is used for identification of cells on grain boundaries and phase boundaries. The grain boundary movement, which affects grain coarsening, is determined by transformation probabilities. The value of those probabilities depends on process and material parameters like temperature and chemical composition. Furthermore fixed values of cell size and time step width are required and have to be defined previously.

The initial microstructure for CA-simulation can be imported from either artificial created microstructure, real micrographs or EBSD-maps. The model output includes mean diameter, grain size distribution and virtually simulated microstructures which can be easily compared with experimental micrographs.

### 4.3 AM3 based multiscale model

From the point of view of the multiscale modeling, the model presented above is relatively simple. There is only downscaling, because the macroscale model is not dependent on the microstructure. However, this problem could be successfully used as an example of AM3.

Numerical models presented above were developed to be used in a "batch mode". The coarse model, which is not dependent of fine scale results, was computed at first. Results (temperature changes in time) were analyzed by the researcher and then microscale models were set up. The microscale models configuration, including its number, locations and properties were chosen manually.

This model was redesigned with AM3. While in the original problem information are passed in only one direction, from macro to microscale, in AM3 based application possibility of both direction communication is assumed. The macroscale model is similar to the original one. The only one difference is removing of stress-strain curve from Deform2D model. For all integration points, stresses are computed inside AM3, basing on material state (strain, strain rate, temperature, time) given by Deform2D model.

Stress computations are delegated from AM3 to one of two fine scale models. The first one is an interpolation of tabularized stress data in dependency of strain, strain rate and temperature. The second model is based on the CA model, described above. Because a stress-strain curve is not dependent on microstructure, interpolation of tabularized data is also used.

### 4.4 Knowledge design

The most important part of the AM3 based model is knowledge. In this case, the most important criterion for model choosing is an existence of a similar model. We expect that results of two fine scale computations in *similar* conditions will give negligibly different results. Efficiency of a whole model could be then improved by neglecting non necessary fine scale models. Criteria of a *similarity* have to be chosen on the beginning. The simplest condition is based on the difference of the temperature $\Delta T$ between the existing models and a probed point. If $\Delta T$ is smaller than given threshold, then a fine scale model is not necessary. Moreover, there is the temperatures range, where particular microscale models can be used. The CA model, described in 4.2 can be applied when the temperature $T$ is between 800°C and 1000°C. When $T$ is lower, no microstructure model can be started, while when $T$ is higher, a high temperature microscale model (which is not present here) should be used. The CA model, when started, will be active, even if the T in this point will fall below lower the temperature threshold. Entire knowledge definition is shown in Figure 2. The knowledge design in this case is relatively simple and should be treated rather as a concept description than a real case solution.

AM3 framework expects from the KBS an answer *which model should be used*. Then a mixed reasoning is only one possible schema.

### 4.5 Results

The KBS was requested to find the proper fine scale model for each time step, for each

finite element. The first CA model had been started in the first time step in the first element (because there were no other CA models). For the following time step it was only one CA model. In the next step, the second fine scale model was started (because existing model was not *similar*). The third and in this case the last CA model was started at time $t = 110$ s. Temperature curves and alpha phase mean grain sizes are shown in Figure 3. Temperature peeks between $t = 200$ s and $t = 220$ s are caused by plastic deformation work. Final microstructures, simulated by CA models in all three steps are shown in Figure 4. Exemplary reasoning session can be seen in Figure 5.

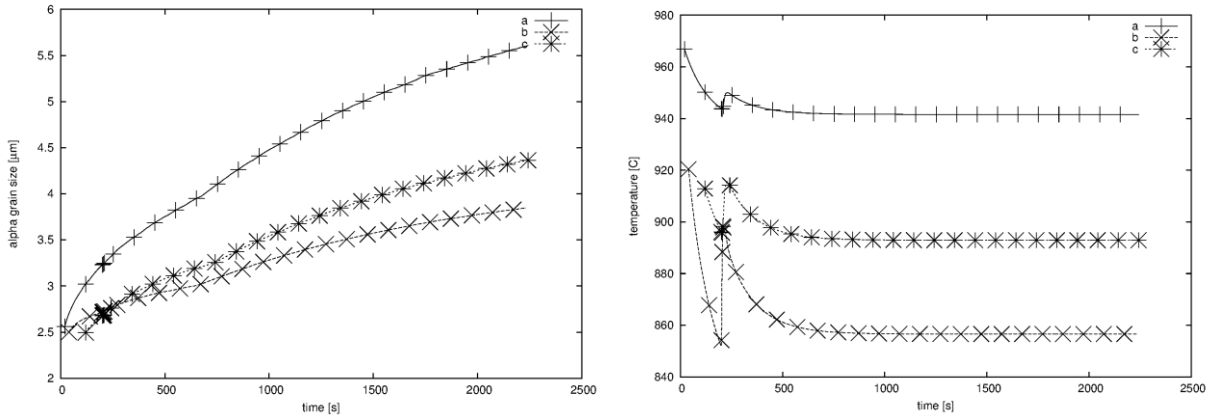
```
TYPES
Models = "CAMicrostructEvolution" , "noMicrostructEvolution" , "HighTempMicrostructEvolution" , "null"
VARIABLES
Temperature: Double; DeltaTemp: Double; isSimilar: Boolean; Model: Models; PreviousModel: Models;
LowerTreshold: Double = 800; UpperTreshold: Double = 1000;

RULE R01
IF PreviousModel = "CAMicrostructEvolution" THEN Model = „CAMicrostructEvolution"
RULE R02
IF Temperature < LowerTreshold AND PreviousModel = "null" THEN Model = "noMicrostructEvolution"
RULE R03
IF Temperature >= LowerTreshold AND isSimilar = false THEN Model = "HighTempMicrostructEvolution"
RULE R04
IF Temperature >= LowerTreshold AND Temperature < UpperTreshold AND isSimilar = false AND
PreviousModel = "null"  THEN Model = „CAMicrostructEvolution"
RULE R05
IF Temperature >= LowerTreshold AND Temperature < UpperTreshold AND isSimilar = true AND
PreviousModel = "null"  THEN Model = "noMicrostructEvolution"
RULE R06
IF Temperature > UpperTreshold AND isSimilar = true  THEN Model = "noMicrostructEvolution"
RULE R07
IF Temperature < LowerTreshold AND PreviousModel = "noMicrostructEvolution"  THEN Model =
"noMicrostructEvolution"
RULE R08
IF Temperature >= LowerTreshold AND Temperature < UpperTreshold AND isSimilar = true AND
PreviousModel = "noMicrostructEvolution"  THEN Model = "noMicrostructEvolution"
RULE R09
IF Temperature >= LowerTreshold AND Temperature < UpperTreshold AND isSimilar = false AND
PreviousModel = "noMicrostructEvolution"  THEN Model = „CAMicrostructEvolution"
RULE R10
IF Temperature >= LowerTreshold AND Temperature < UpperTreshold AND PreviousModel =
HighTempMicrostructEvolution"  THEN Model = „CAMicrostructEvolution"
RULE R11
IF DeltaTemp < 30  THEN isSimilar = true
RULE R12
IF DeltaTemp >= 30  THEN isSimilar = false
```

**Figure 2**: Rules for chosing of the fine scale model for thermo-mechanical treatment of Ti-6Al-4V

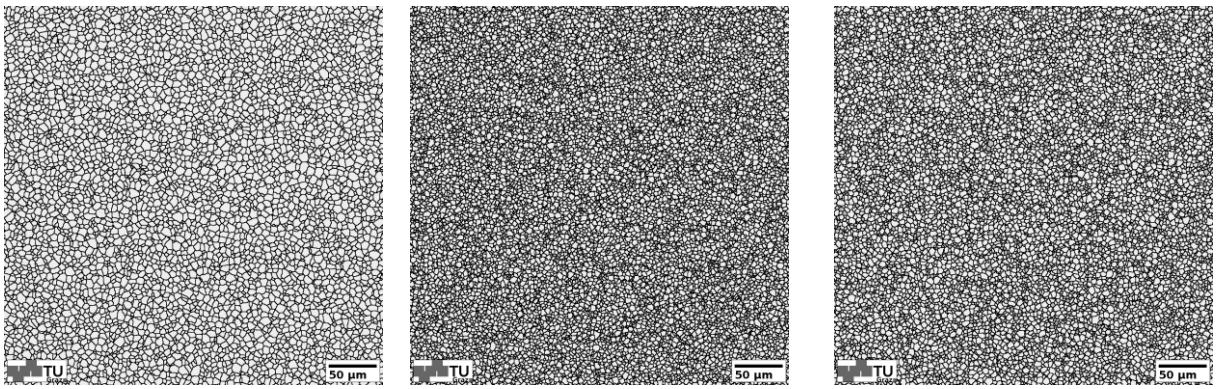
## 5 CONCLUSIONS

The methodology presented in this paper allows the adaptation of the multiscale model with use of knowledge. Due to unification of interfaces and some algorithms it also simplifies development of new multiscale models. Thanks to that, the researcher can work on higher level of abstraction. However, it has to be remembered that increasing of an abstraction level almost always leads to decreasing of efficiency. Therefore, described methodology is not competitive with mathematically consistent solutions cited in Introduction. Dedicated solution with strong mathematical background will be probably more efficient and accurate than general one. However, in many cases generality, ability of predicting additional phenomena and ease of use can be more important than numerical efficiency.




alpha grain size [$\mu m$] temperature [$°C$]

**Figure 3**: Alpha phase grains sizes and temperatures for CA simulations




(a) (b) (c)

**Figure 4**: Simulated microstructures at time t = 2000s for *a*,*b* and *c* CA simulations

Presented example is relatively simple. It can be improved with adding more fine scale models types, making *similarity* more precise (e.g. dependent on temperature history, not only actual value) etc.

Rules for additional phenomena detection can be added to KB. It is possible to have rules also for phenomena, which cannot be modeled (there is no suitable fine scale model). In such case, while of course effects of such phenomena cannot be taken into consideration, neglecting of them will be signalized by KBS.

```
start
final_variable_set [Model]
source_variable_found [PreviousModel]
source_variable_value_set [PreviousModel]; [“null”]
rule_found_by_premise [PreviousModel]; [R01]
rule_evaluation_result [R01]; false
rule_found_by_premise [PreviousModel]; [R02]
variable_value_needed [Temperature]
rule_found_by_conclusion [Temperature]; [null]
source_variable_value_set [Temperature]; [800]
rule_evaluation_result [R02]; false
rule_found_by_premise [Temperature]; [R07]
rule_evaluation_result [R07]; false
rule_found_by_premise [Temperature]; [R10]
rule_evaluation_result [R10]; false
rule_found_by_premise [Temperature]; [R04]
rule_found_by_premise [Temperature]; [R05]
variable_value_needed [isSimilar]
rule_found_by_conclusion [isSimilar]; [R11]
rule_found_by_conclusion [isSimilar]; [R12]
variable_value_needed [DeltaTemp]
rule_found_by_conclusion [DeltaTemp]; [null]
source_variable_value_set [DeltaTemp]; [2000]
rule_evaluation_result [R12]; true
conclusions_value_set [isSimilar]; [false]
final_variable_idntified [Model]; false
rule_evaluation_result [R05]; false
rule_evaluation_result [R04]; true
conclusions_value_set [Model]; [“MicrostructureEvolution”]
final_variable_idntified [Model]; true
end
```

**Figure 5**: A trace of exemplary reasoning

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