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Processes simulations with multiscale materials models using a dedicated interface

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Abstract

The main goal of this work is the integration of in-house software with commercial numerical software based on the finite element method (FEM). The main idea is to develop a universal interface to perform process simulations with multiscale models. The interface allows the combination of external procedures with commercial software with minimum programmer's work putting in integration. As an example, the model of material recrystallization of steel was implemented, added to the commercial application, and the software was tested for a process defined as a sequence of compression and cooling. The material model takes into consideration each type of recrystallization that occurs during a sequence of thermal and mechanical processing such as static recrystallization (SRX), dynamic recrystallization (DRX), and meta-dynamic recrystallization (MDRX). It allows the prediction of recrystallized volume fraction (X) and grain growth on each step of numerical simulation for each Gauss point in the computation domain. The presented multiscale model of process sequences not only allows to calculate microscale model parameters such as grain growth and recrystallized volume fraction, but also reflects the impact of the microscale model on macroscale parameters.

Keywords: multiscale modelling, material models, models integration, recrystallization

1. Introduction

Rapid technological progress means that the mechanical and thermal properties of products need to be constantly improved. The final product must fulfill strict quality requirements and also comply with the safety requirements and environment protection regulations. Industrial production requires constant material properties of each manufactured piece of product. This can be accomplished by detailed control of the production process. Products with similar microstructure parameters have similar mechanical properties, meaning that by controlling the microstructure during the manufacture, specific parameters of final products can be obtained. Microstructure development is controlled by a proper combination of strain and temperature during deformation.

For more than a half a century, many scientific publications have been published on microstructure evolution during recrystallization. Sellars (1985, 1990) and co-workers at the University of Sheffield were pioneers in the field of modelling microstructural evolution during hot rolling. The other major research centers involved in microstructure model development are Kawasaki Steel, where Saito et al. (1980) modelled controlled rolling and cooling after hot rolling to obtain the optimal mechanical properties of plain-carbon steels. At Nippon Steel Senuma and Yada (1986) applied Avrami expression for dynamic recrystallization kinetics for single-peak flow cures. More recently, the most important contributors in

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development models of dynamic recrystallization have been Jonas (1996) in Canada, Sellars (1990) in the UK, Sakai (1995) in Japan and Hodgson (1993, 2004) in Australia. The summary of numerical models of recrystallization was described, i.a., by Madej et al. (2016).

The main goal of the authors' work is to present the ways to combine analytical models of microstructure evolution with commercial software based on a numerical approach, especially FEM. This requires particular microstructure development model input, the available outputs, and the ways of integration. Here, the authors focus on results' analysis obtained with their own software implementation and that of of FEM software using a user subroutine. To present the challenges which must be solved during such an integration, two pieces of commercial FE software were analysed: Larstran PEP and Abaqus FEA.

2. Multiscale numerical modelling

Numerical modeling is commonly used in scientific work and also by engineers in industrial research. In industrial manufacturing, it can significantly reduce costs. Such an approach finds application in solving numerous problems, which requires developing new numerical models becoming now more and more complex. The multiscale approach assumes that every problem can be represented by a hierarchical model for further investigations of the mechanism taking place in it. Many problems in nature involve multiple active scales, and solving the major problem requires the division of time or space scale into many minor problems. Various numerical models that solve individual problems are combined in one simulation and construct one concurrent multiscale model. These models are the most complex and complicated in implementation because the results of one model have an influence on results to another during the whole time of the process. Multiscale models are constantly developed, and a lot of scientific publications, can be found in this area. They are comprehensively described in the works of Steinhauser (2008) and E (2011).

Multiscale models were divided into two families by E. The first one is homogeneous, where models form a single set of equations over the time and spatial scales. In many practical cases solving problems in all scales with a consistent set of differential equations is not possible. The second family is heterogeneous; it consists of independent sub-models described in different scales that pass information between themselves in different ways and conditions. In this work, the second type of approach was used, i.e., Heterogeneous Multiscale Modelling (HMM) proposed and described by E (2011).

3. Division of calculation domain

Preparation of a multiscale model requires two major decisions to be taken. The first of these is the manner of the computational domain division. In the HMM model, two types of domain division are proposed: Type A and Type B that assume integration coarse and fine-scale models, respectively, at the region of singularity, presented in Figure 1, and at the whole computational domain in each integration point of Fine Element mesh, what is presented in Figure 2.

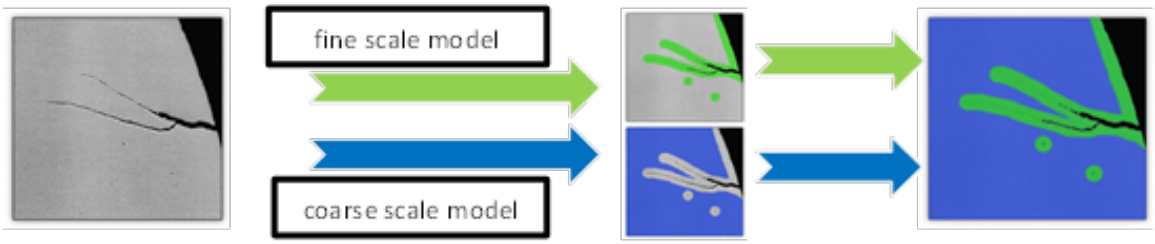

Fig. 1. Computational domain division, Type A

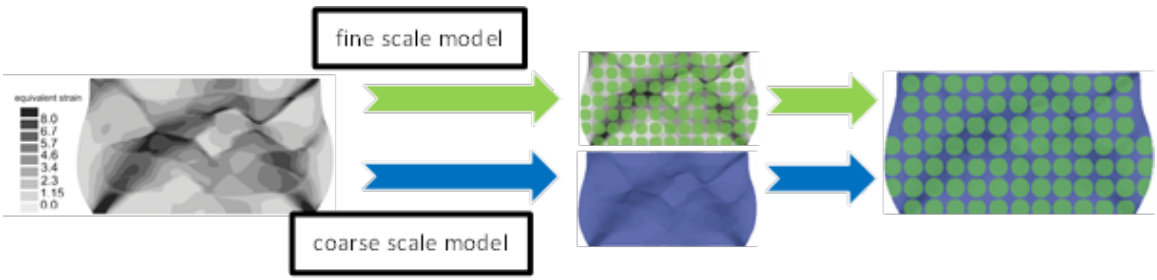

Fig. 2. Computational domain division, Type B

Type A

This class of problems deals with local defects problems and singularities such as shocks and dislocations where macroscale is suitable for a major part of the physical domain, and the microscale model is only necessary at the singularity region.

Type B

The second class of problems is used when the macroscale model needs to be supported by the information from the microscale scale. There are no regions of interest in this approach and the calculation of coarse and fine models needs to be processed in the whole calculation domain.

That division of problems generates a problem of parameters passing between models. The most common approach for Type B is to integrate both micro and macro models and process the calculation in the whole domain. Type A needs to cope with the interface on the boundaries of both models. If models' integration points do not overlap, micro-macro parameters need to be interpolated.

4. Parameters transfer

The second problem of multiscale model development is the way and the sequence of parameters transfer between models that have to be determined. Sequential coupling requires separate calculations for coarse and fine-scale models and transfer parameters from one to another in a specific form. The results set of data from one model is the input data for the second model. There is no time correlation between numerical models in this approach, and the first model can exist as a solution to an individual problem. Data from one scale can be transferred to another scale problem in pre-processing, which is presented in Figure 3. Those kinds of numerical models are used as extensions or continuations of the available results because the outcome of the new numerical simulation does not affect the previous simulation.

The second approach is to continuously transfer parameters during simulation between fine and coarse models. Results of one scale model influence another, and numerical simulation cannot be calculated separately because of continuous data transfer, as it is presented in Figure 4. This approach requires access to all parameters in each of the solving scale problems on the implementation level what is not always provided by numerical software engineers.

Another challenge to cope with is the dependence between a number of scales in HMM and computer power demands. Every extra scale model increases computer power demands exponentially. Thus, a compromise has to be found between the accuracy of the results and the time available to obtain them.

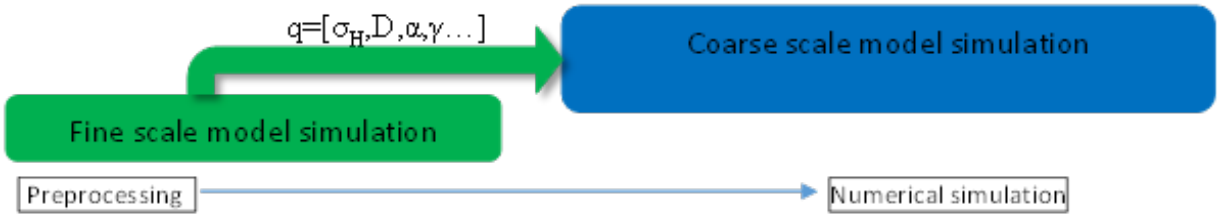

Fig. 3. Parameters transfer, uncoupled model

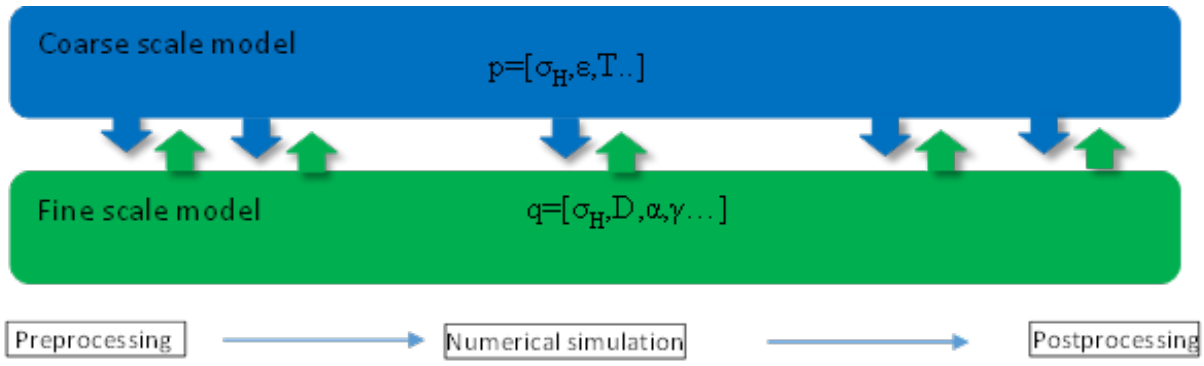

Fig. 4. Parameters transfer, coupled model

5. Integration issues

The most common approach in scientific research is to analyze and process results of numerical software of coarse-scale to develop a multiscale model. Such a sequential model allows the generation of a numerical model of the same or another scale but is burdened with many restrictions such as data limitation. Input data are correlated with finite elements coordination, node or element. If the transferred parameters do not overlap the new model's coordinates, their values are interpolated or approximated before transferring them to upscaling or downscaling model.

Many commercial numerical software allows their functionality to be extended with user procedures. That approach permits the implementation of new functionalities into FEM software, but it requires the installation of a compiler if it is not provided. User subroutines can exchange used equations such as flow curves or extend functionalities of the software to calculate, for example, microstructure evolution model if the model is not provided.

Abaqus software allows for the implementation of one's own procedures in, e.g., Python and running them as a sequential model using an inner interpreter. Such a method of calculation provides access to the whole set of data stored in Finite Element mesh but, as was described above, the results cannot affect the calculation of the first scale model. To develop the coupled model, it is necessary to use one of the provided subroutines like UMAT or UHARD. These subroutines have different applications and require a different set of initial data. Subroutines are implemented in the Fortran language, i.e., basic programming skills on the part of the user are necessary.

Larstran PEP software not only allows the implementation of user subroutines in Fortran to develop a coupled multiscale model but provides the opportunity to modify solver files to extend its functionalities. These subroutines are added to a specific simulation and compiled as an integrated part of the model. Larstran PEP software exports data in many files formats. That gives an opportunity to integrate models in sequential calculations with other FEM software that imports this file format.

In this work, the connection of Larstran-PEP software's macroscale model with in-house microstructure evolution software to develop the multiscale sequential model of multistep hot strip rolling schedules both in pre and post-processing is presented.

6. Implemented multiscale model

The multiscale material model requires the definition of sub-models like yield stress model for macro model and microstructure model for microscale. Each of the models is described by the parameters, which have to be identified for a specific material. The identification is performed based on the results from classic material tests.

7. Macroscale model

Implemented model of yield stress in Larstran PEP software is based on the Hansel–Spittel equation of the form:

$$\sigma_p = A_1 \varepsilon^{A_2} \exp(A_3 \varepsilon) \dot{\varepsilon}^{A_4} \exp(A_5 T) \tag{1}$$

where: σ_p – yield stress, ε – effective strain, $\dot{\varepsilon}$ – effective strain rate, T – temperature [K].

Parameters for the yield stress model were determined based on the axisymmetric compression test. Results of the parameters identification are shown in Table 1.

Table 1. Yield stress parameters

Parameter				
A_1	A_2	A_3	A_4	A_5
10539	0.435	−0.7888	0.1118	−0.00355

8. Microscale model

The microstructure evolution model is based on the Avrami equation describing the kinetics of recrystallization. Implemented models coupe with three types of recrystallization during whole cycles of material processing. For compression, a microstructure model that includes dynamic recrystallization phenomena is implemented. After compression, when cooling takes place, the model of microstructure evolution with meta-dynamic and static recrystallization is used.

Static recrystallization

The recrystallization condition is based on strain value. A certain minimum threshold of strain needed to initiate the static recrystallization is assumed at $\varepsilon_{cr\text{-}SRX} = 0.03$. The classic Avrami equation for recrystallization volume fraction X is used (Sellars, 1985):

$$X = 1 - \exp\left[-0.693\left(\frac{t}{t_{50}}\right)^n\right] \tag{2}$$

where: n – Avrami exponent, t_{50} – basic time for 50% recrystallization.

Time for 50% recrystallization depends on the following parameters: strain, strain rate, temperature, and grain size prior to recrystallization. The following commonly used equation to calculate t_{50} (Sellars, 1990) was applied:

$$t_{0.50} = A\varepsilon_i^{-a1}\dot{\varepsilon}^{-a2}D_0^{a3}\exp\left(\frac{Q_{SRX}}{RT}\right) \tag{3}$$

where: ε_i – effective strain, $\dot{\varepsilon}$ – effective strain rate, D_0 – grain size prior to recrystallization, T – temperature [K].

The grain size after static recrystallization is calculated from the following equation:

$$D_{SRX} = B\varepsilon^{b_1}\dot{\varepsilon}^{b_2}D_0^{b_3}\exp\left(\frac{Q_{SRX}}{RT}\right) \tag{4}$$

The coefficients in equations (3) and (4) were obtained based on the experimental test. In literature, there can be found two tests: stress relaxation test and two-step compression test used for that purpose. Identified parameters for the kinetics equation and grain size equation are presented in Table 2.

When partial static recrystallization takes place, some retained strain remains in the material. The initial strain for the next simulation is calculated as:

$$\varepsilon_{k+1} = W\varepsilon_k\left(1 - X_{SRX}\right) \tag{5}$$

where: ε_{k+1} – retained strain at the exit to the next pass, ε_k – effective strain in the previous pass, W – coefficient with value 1, but some researchers use it to account for the influence of the recovery.

9. Multiscale model

Implementation of the multiscale model was performed by the connection of FEM Larstran PEP and in-house implemented program for microstructure evolution with recrystallization phenomena included. The connection between models via files saved in the Patran file format was defined. That file format can be exported and imported by Larstran and interpreted and generated by authors' implemented software.

Implementation of the microscale model was performed in Python in version 3.5. This language is a high-level interpreted language that can be easily modified with good readability of code for non-programmer researchers. The major advantage of Python is independence from a particular operating system; its cross-platform nature allows the use of the same source code in Windows and Linux based operating systems. Python e is being constantly developed and increasingly commonly used in numerical simulations.

The approach is defined by the combination of external specific file format and procedures implemented in the Python language forms interface, which can be applied to connect any models in various scales, implemented both as commercial and in-house software.

10. Example of computations

To present the possibilities of the developed approach, the process of sequential compression and cooling was selected as an example. Simulation of macroscale model was performed in Larstran and Abaqus for a symmetric sample of 15 mm height, 20 mm width, and 35 mm length with initial temperature 1200°C and homogeneous grain size of 80 μm. The tool dimension was 10 mm in width and 40 mm in length. The scheme of the input model is presented in Figure 5.

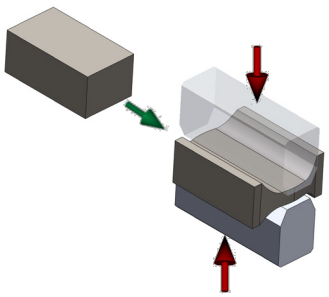

Fig. 5. The geometry of the sample and schematic deformation of plastometric test

The whole model of the multistep process was divided into six stages with compression and cooling sequences. The process of multistep compression with temperatures and strains is presented in Figure 6 as variant 2.

Table 2. Coefficients in microstructural equation for static recrystallization

Static recrystallization (SRX)	1.53	2.1E-11	3.6	0.3	0.637	205000
	n	A	a_1	a_2	a_3	Q_{SRX}
	1.487	0.055	0.08	0.88	8172	–
	B	b_1	b_2	b_3	Q_{SRX}	–

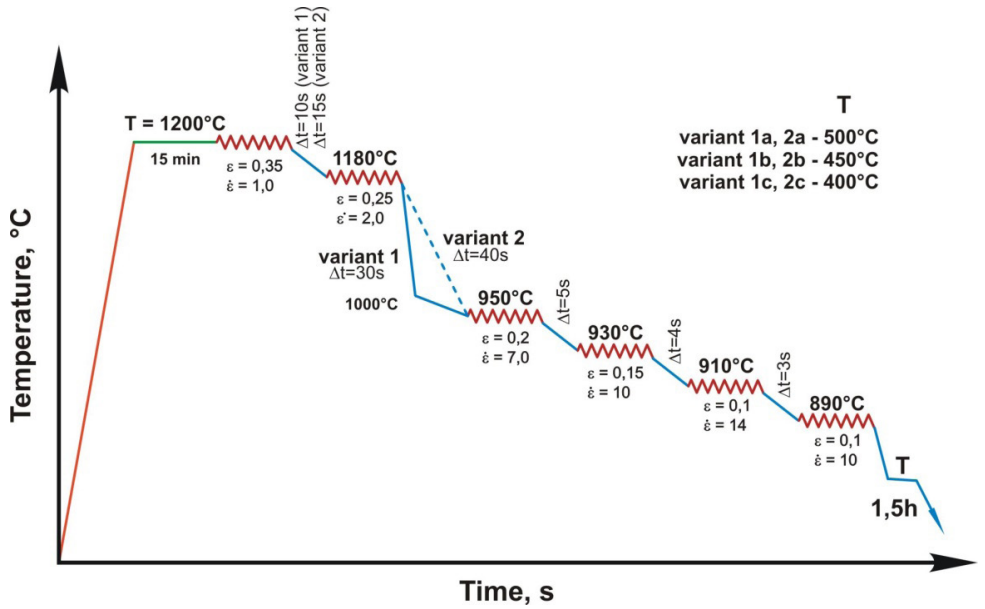

Fig. 6. Scheme of deformation and heat treatment

The calculation of the multiscale model is performed sequentially, and the results of each macroscale model are the input data for microscale model. The results from the microscale model of recrystallization fraction had an influence on initial macroscale strain according to Equation (5).

During compression, the model includes dynamic recrystallization in terms of effective strain value. If effective strain value is greater than the critical value calculated by Equation (6) the recrystallized volume fraction (X_{DRX}) is calculated:

$$\varepsilon_{cr\_DRX} = p_1 D_0^{p_2} Z^{p_3} \tag{6}$$

where: Z – Zener–Hollomon parameter defined as:

$$Z = \dot{\varepsilon} \exp\left(\frac{Q_{DEF}}{RT}\right) \tag{7}$$

Recrystallized volume fraction in dynamic recrystallization is the function of strain:

$$X_{DRX} = 1 - \exp\left[-p_7\left(\frac{\varepsilon - \varepsilon_{cr\_DRX}}{\varepsilon_s - \varepsilon_{cr\_DRX}}\right)^{p_8}\right] \tag{8}$$

where: ε_s – saturation strain calculated from the equation:

$$\varepsilon_s = p_4 D_0^{p_5} Z^{p_6} \tag{9}$$

If X_{DRX} exceeds a value 95%, full dynamic recrystallization is completed, and grain growth is calculated. When the time of recrystallization is shorter, and X_{DRX} is below 95% the remaining volume fraction X_V is calculated for meta-dynamic recrystallization by the following equation:

$$X_V = 1 - X_{DRX} \tag{10}$$

When metadynamic recrystallization occurs, the grain size is calculated as a weighted average of the grain size after dynamic recrystallization D_{DRX} (11) and final grain size at the end of the metadynamic recrystallization D_{MDRX} (12) by the Equation (13).

$$D_{DRX} = p_9 Z^{-p_{10}} \tag{11}$$

$$D_{MDRX} = q_4 Z^{-q_5} \tag{12}$$

$$D_1 = D_{DRX} X_{DRX} + D_{MDRX}\left(1 - X_{DRX}\right) \tag{13}$$

The whole sample was meshed in Larstran-PEP software, and the calculation domain was divided initially into 1309 nodes for the first compression up to 2108 in the last compression step. Because of mesh deformation, at the beginning of each next step, the calculation domain needed to be remeshed with the data transfer procedure.

After calculation of model in microscale, in-house software generates two types of data: for Larstran-PEP post-processing for visualization of recrystallized volume fraction and input data for the next step pre-processing.

Results from the microscale model, recrystallized volume fraction, and grain size, after the first compression are presented in Figure 7 and Figure 8. Data from the cross-section in the center of the sample is shown.

From every simulation, seven points of interest at the cross-section were selected to investigate the microstructure evolution according to the schema presented in Figure 9.

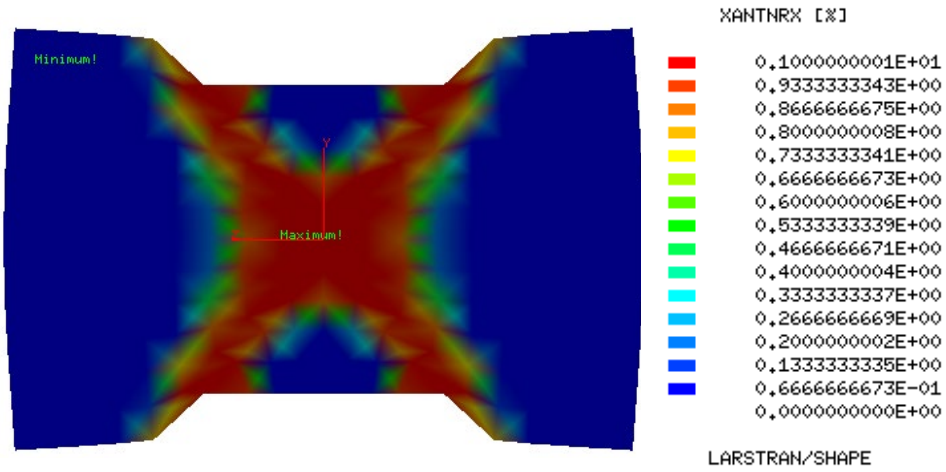

Fig. 7. Recrystallized volume fraction after the first compression

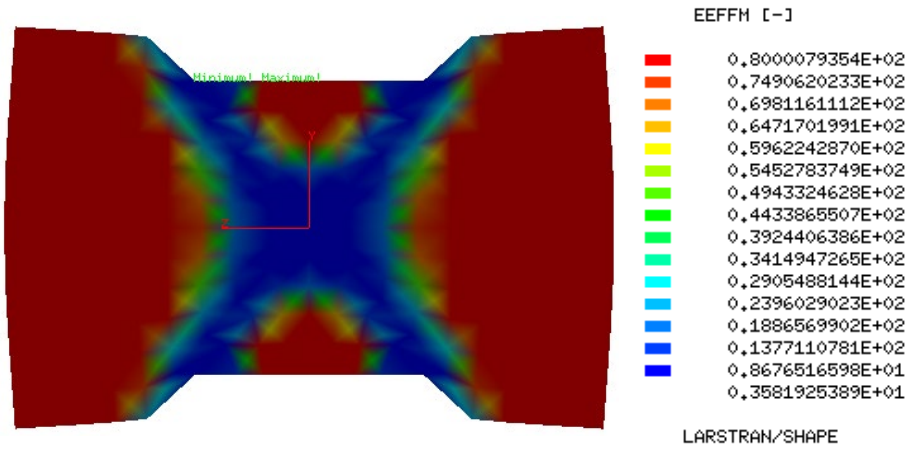

Fig. 8. Grain size after first compression

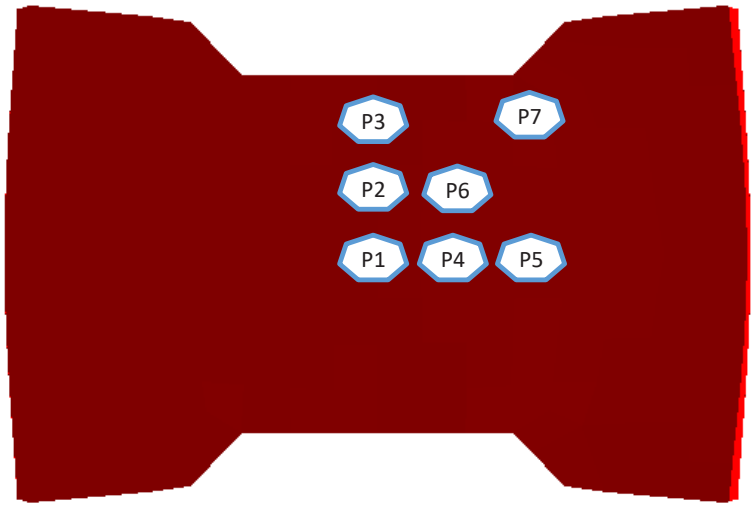

Fig. 9. Points of interest at the cross-section of the sample

Such a location allows the investigation of microstructure evolution at points with different strain and temperature values. A diagram of the grain size during first pressing is presented in Figure 10.

The same set of data is calculated during the cooling process after the compression. During cooling in the points where dynamic recrystallization is not completed, meta-dynamic recrystallization phenomena occur in the remaining volume. In the points where strain value did not pass the critical value of DRX, static recrystallization occurred. The results of the model calculated in microscale are presented in Figure 11.

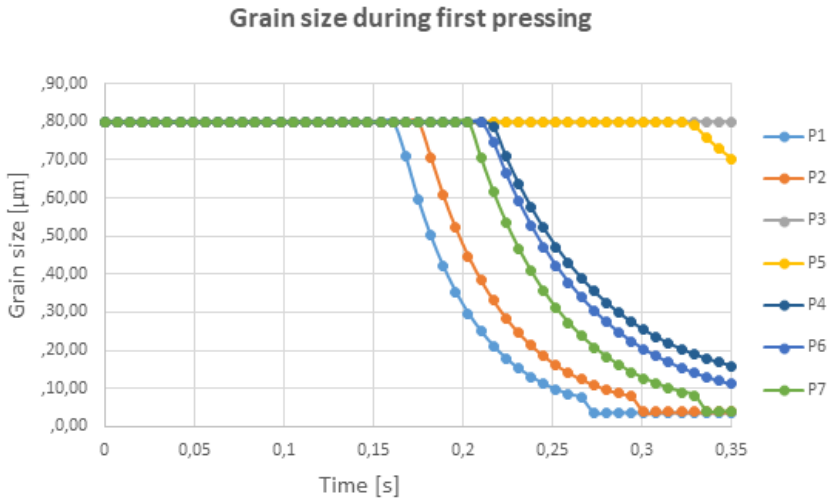

Fig. 10. History of grain size during the first compression in the points of interest marked in Figure 9

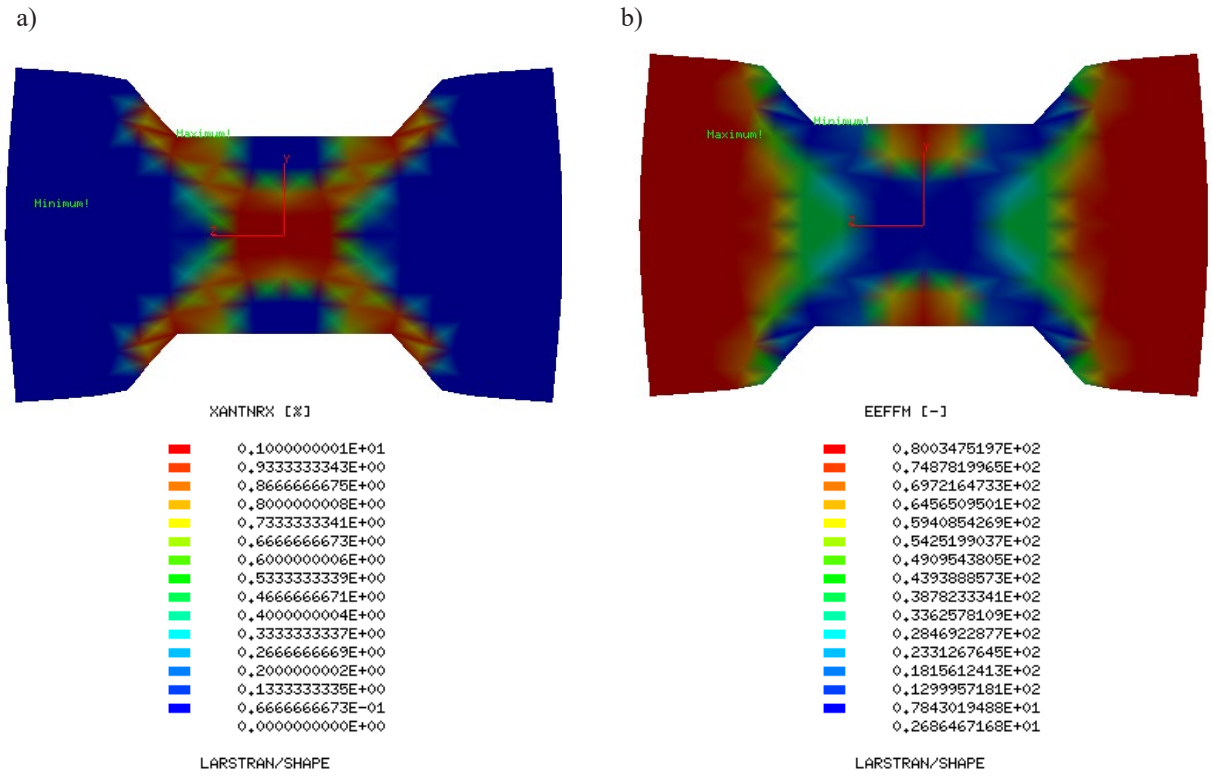

Fig. 11. Recrystallized volume fraction and grain size at the end of first cooling: a) recrystallized volume fraction; b) grain size

The selected points were located in the same scheme at the cross-section of the sample, and the history of microstructure evolution in presented in Figure 12.

Results of the cooling simulation are input data for another step of compression. The remaining strains are calculated according to Equation (5) (Fig. 13).

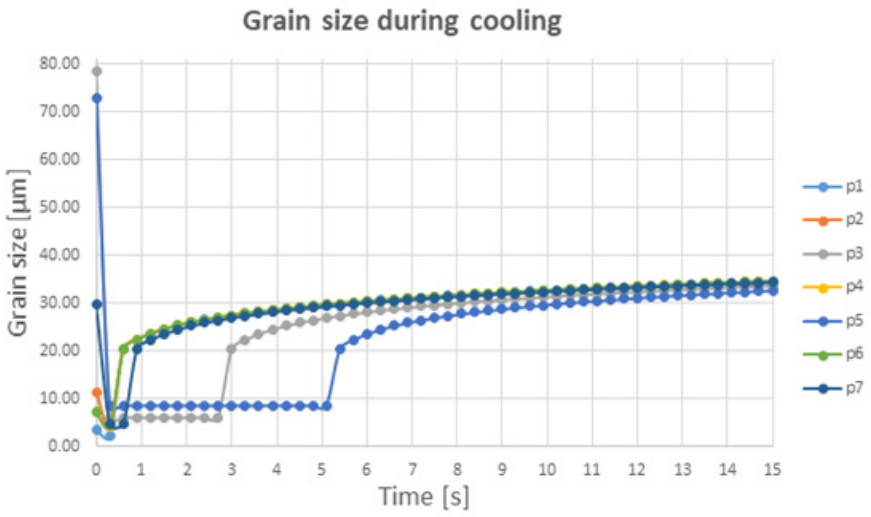

Fig. 12. Grain size history during first cooling for seven points of interest

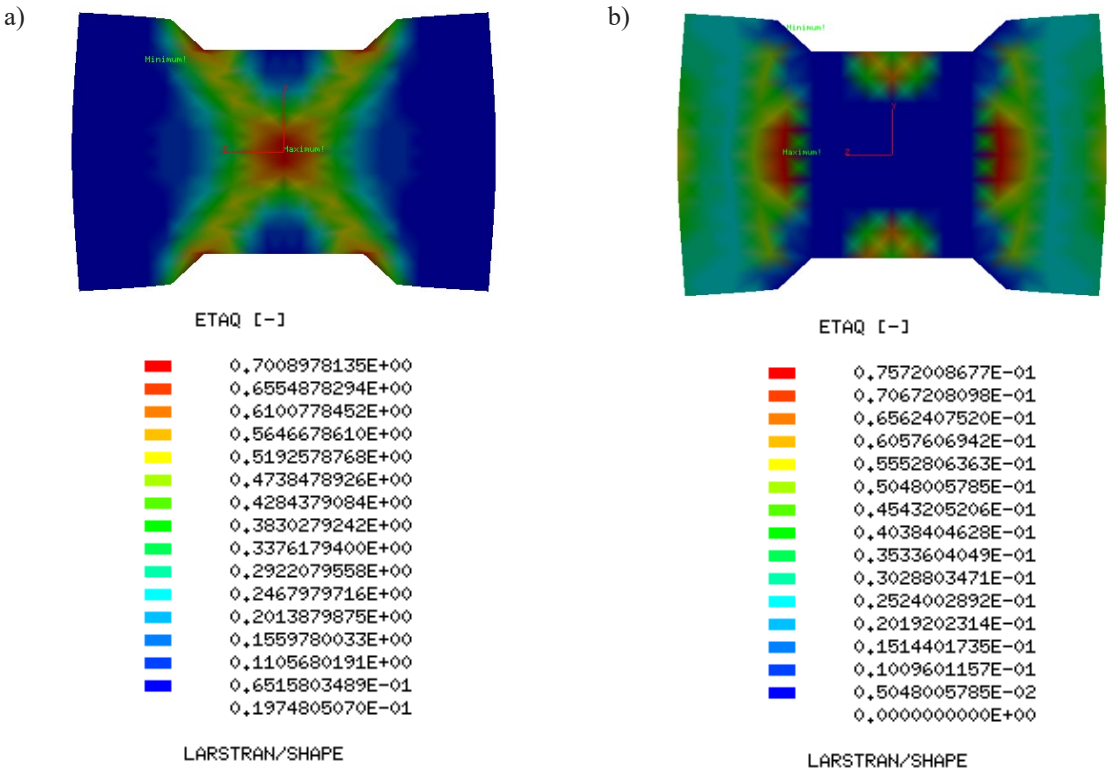

Fig. 13. Strain differences before and after considering the remaining strain at the beginning of the second compression: a) strain; b) remaining strain included

The whole process is performed for every stage of the process, and results for the first point in the center of the sample are presented in Figure 14.

Calculations were performed using a PC computer equipped with 8-core 64-bit processor Intel Core i7-4770 and 16 GB RAM. Calculation times were strictly dependent on the process step and solver used. The time required to calculate a simulation based on the thermo-mechanical solver used for compressions was in the order of 2 h to 8 h. Calculation times were strongly dependent on the number of elements and deformation ratio. Simulations of cooling based on thermal solver were calculated much faster – from 5 min to 20 min. That time was depended on the cooling time used in the process. Microstructure evolution model implemented in Author's software based on macro-model data from FEM software were calculated in 30 s to 60 s. That time was depended on the number of elements and type of phenomena that occur during the process like DRX, MDRX, or SRX.

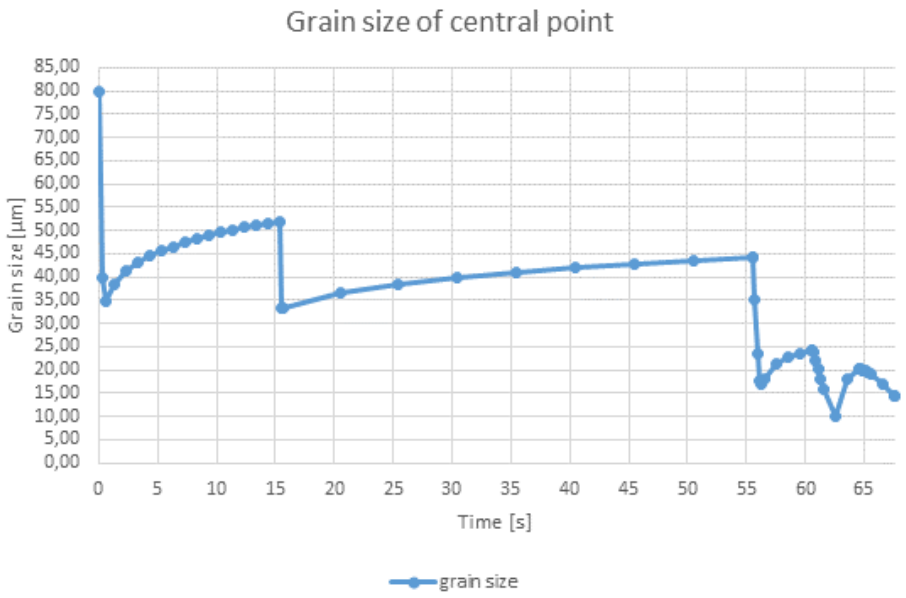

Fig. 14. Grain size history for the whole process for the point in the sample center

The whole procedure of data transfer was repeated in Abaqus software and applied to the first cycle of compression and cooling sequence with the same in-house procedures for microstructure evolution, and the results were comparable.

11. Conclusions

In the work, an application of the universal interface dedicated integration of models implemented in various software was discussed. The interface module is based on independent files and subroutines, which allow to the exchange of information between software and models. As an example, a multistep compression and cooling process was selected to perform computations. The obtained results are consistent with the available data in the literature.

It was shown that the implementation of correct interfaces allowed the use of external procedure, e.g., a material model, in commercial FEM software and to compute the numerical simulation results in post-processing as well as to expand the software functionalities and perform coupled multiscale simulations. Interface adaptation allowed to include the same model into various software with no model code modifications. The approach allows the usage of highly complex models with their internal optimization and data frow. There is no need to make time consuming process of full model's code understanding in order to adapt it to the specific FEM software with its individual sub-routines requirements, only the implementation of the corresponding interface is required.

Acknowledgements

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