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SPROC – SMART PROCESS CONTROL TOOLKIT FOR SEMI -FINISHED PRODUCTS MANUFACTURING

*J. Kronsteiner and E. Kabliman

LKR Leichtmetallkompetenzzentrum Ranshofen GmbH, Austrian Institute of Technology, Lamprechtshausenerstr. 61, 5282 Braunau am Inn - Ranshofen, AUSTRIA

*(*Corresponding author: johannes.kronsteiner@ait.ac.at)*

ABSTRACT

In the present work, we developed a Smart Process Control Toolkit (SProC) as a single simulation environment for the modelling of materials microstructure and its interaction with the local microchemistry during manufacturing of semi-finished products. This toolkit supports the data communication between sub-sequent processing steps such as casting, homogenization, pre-heating to deformation, etc. The thermo-kinetical simulation software MatCalc of MatCalc Engineering© GmbH was used for modelling of precipitation kinetics, such as formation of primary and secondary phases and their evolution. An import/export functionality of the precipitation distribution after each processing step was implemented to follow the parameter history. For the evolution of the local microstructure, a Mean Dislocation Density based Model (MD^2M) was used. This model consists of two parts: (1) Flow Stress Model for calculation of the total strength during the deformation and (2) Static Recrystallization Model for account of the recrystallization and grain growth after the deformation. Validation was done by a comparison of experimental and simulated hot compression tests of a conventional AA2024 alloy.

KEYWORDS

Through process modelling, Microstructure, Microchemistry, Mean dislocation density model, Data management

INTRODUCTION

Optimization of a semi-finished products quality, elimination of typical production issues and cost savings are of a great demand for supply industries. However, it is currently not feasible to investigate the whole manufacturing process in detail at an industrial level. Concerning the processing parameters, one must understand the correlation mechanisms between macroscopic properties and microscopic material behavior. Numerical simulations, which could reproduce the real processing conditions on the one hand, and employ a physically based modelling on the other, are thus attracting a lot of attention and their power is no longer under the question. It is well known that e.g. the total strength of the material depends directly on distribution of precipitation particles and mean grain size. In order to follow their evolution during the manufacturing process beginning from casting to the final semi-finished product, and thus be able to control the process, one should use the techniques which would at the same time reproduce experimental processing conditions of real size objects (e.g. sheet, extrusions, etc.) and account for the evolution of a local microstructure and its interaction with the microchemistry. A commonly used approach is to implement a model which would describe the evolution of microstructure based on a dislocation density approach into a user defined material subroutine of some finite element solver. There is, however, also an influence of the manufacturing process by e.g. the evolution of a local microchemistry (formation, transformation and dissolution of the precipitation particles) on the microstructure and thus the macroscopic material behavior. Thus, a method is needed to follow the variable history through the simulation of the whole production chain.

In present work, we developed a single simulation environment, which includes:

- integration of a microstructure model based on the mean dislocation density (MD^2M) into a finite element solver LS-DYNA®,
- linking between a thermo-dynamic modelling of the phase kinetics performed by the MatCalc software and the thermo-mechanical material model in LS-DYNA®,
- automatic data exchange between numerical simulations at subsequent processing steps.

This simulation environment is then called Smart Process Control Toolkit (SProC), which should allow the user to control the microstructural properties through the whole production chain (see Figure 1).

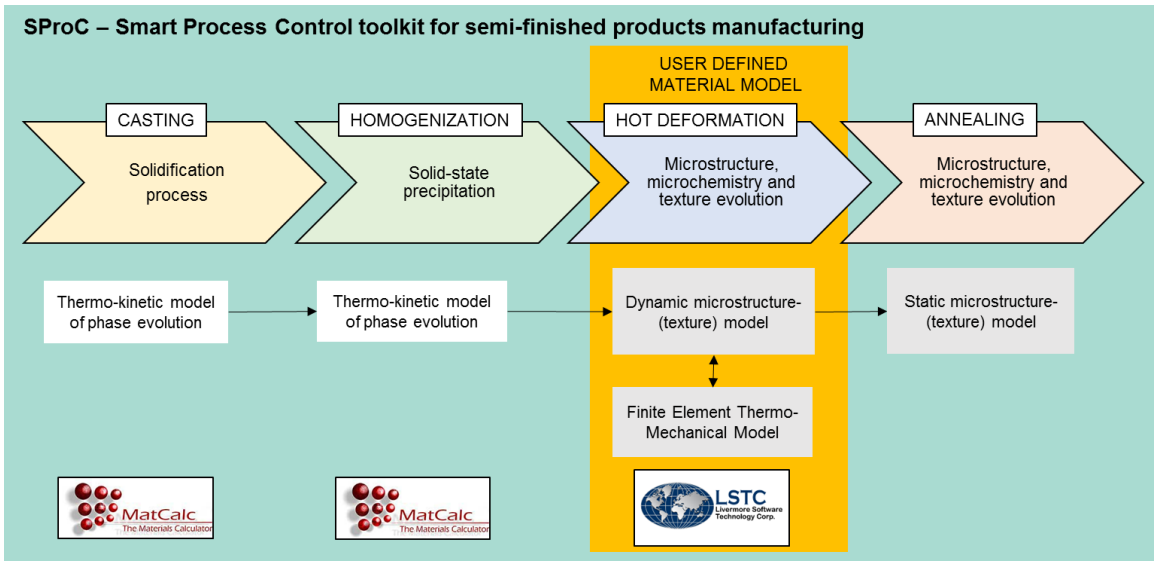

Figure 1. A concept of Smart Process Control Toolkit (SProC).

For demonstration purposes, we choose hot compression tests of a conventional AA2024 alloy, which consist of relevant production steps before the deformation such as casting, homogenization, heat treatment to a deformation, single step deformation and post deformation annealing. The results are then validated by corresponding experimental trials using the deformation dilatometer (DIL 805 A/C of Texas Instruments). Applying this procedure should allow to get a better insight into the evolution of the local microstructure and its interaction with the local microchemistry during the thermo-mechanical processing and to improve the prediction accuracy of the macroscopic material properties.

SMART PROCESS CONTROL TOOLKIT (SPROC)

In order to perform a Through Process Modelling (TPM) in a single simulation environment, a main control software to govern the data exchange and different file manipulation tasks is necessary. The developed toolkit (SProC) presented in this work is not only intended to control the whole process simulation, but it also provides a single framework to distribute information between two major input files (master and process) and all sub-processes. This approach helps to minimize sources of potential errors from user inputs. The necessary steps for preparing a single TPM simulation are illustrated in Figure 2.

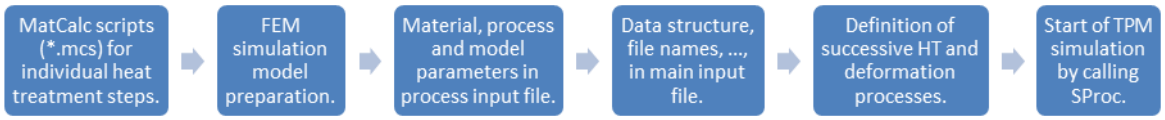

Figure 2. Preparation of a single TPM simulation.

At the point in time when a process is prepared, SProC collects the necessary data from the input files and provides the individual processes with the relevant values using wildcards. In the case of MatCalc, a main input file (0_main_run.mcs) is prepared. This script contains information about the used databases, the chemical composition of the studied material, the relevant phases and heat treatment variables, which are setup from the main input file (master-input.cfg) by using SProC. This MatCalc main input file is afterwards used for each individual MatCalc script (casting.mcs, hom-ht.mcs, pre-ht.mcs, etc., …) to simulate the casting, homogenization, heating to a deformation temperature etc. correspondingly. If modifications due to intermediate results are necessary, the file is adapted for the following process. The precipitation matrixes and phases are defined in separate MatCalc scripts “mc_matrix.mcs” and “mc_phases.mcs”. The data transfer of the precipitate distribution during the MatCalc simulation from one production step into the next one is realized by the commands “export-precipitate-distribution” and “import-precipitate-distribution”. It is also possible to calculate user-defined functions on-the-fly by calling a MatCalc script “mc_functions.mcs”. The structure of the MatCalc scripts and simulation setup is kept as general as possible for easier usage in case of different alloys or thermo-mechanical processing.

A special remote-control program, called MCR, provided for the execution of MatCalc by a third-party software (herein SProC) is used to load and control the individual scripts for the heat treatment processes. Based on a named pipe, commands can be transferred directly between a third-party software and MatCalc. Only one single MatCalc session is started at the beginning of a new TPM simulation, while the individual MatCalc scripts are then called via MCR from within SProC based on the process sequence defined in the process input file. It is thus possible to load pre-defined MatCalc scripts, start corresponding calculations and export output data remotely. Creation of working directories and data handling between subsequent processes simulations are handled again by SProC. Since the MatCalc session is kept open, all the relevant databases and the history results are available for a subsequent simulation of the next production step. Thus, a time-consuming data exchange between a third-party software and MatCalc can be minimized.

During simulation of a deformation step the temperature and strain rate values are directly transmitted from the LS-DYNA® solver to MatCalc. As respond the information about microchemistry (fraction of nano-sized particles and solute atoms in the Al-matrix) is received. This data is then transferred

by SProC to a microstructure model (MD²M) implemented in present work into a user defined material subroutine of LS-DYNA®. This model is based on evolution of mean dislocation density and is used for description of the total strength during the deformation (Flow Stress Model) and the static recrystallization after the deformation (Static Recrystallization Model) as described in Sherstnev, Lang, and Kozeschnik (2012), Kabliman and Sherstnev (2013), and Kabliman, Sherstnev, Kronsteiner, and Ebner (2014).

The evolution of mean dislocation density is considered as dislocation production and their reduction through spontaneous annihilation and thermally activated climb:

$$\frac{d\rho}{dt} = \frac{M\sqrt{\rho}}{b \cdot A}\dot{\varphi} - 2B\frac{d_{ann}}{b}\rho M\dot{\varphi} - 2CD\frac{Gb^3}{k_B T}\left(\rho^2 - \rho_{eq}^2\right) \tag{1}$$

Here *A*, *B* and *C* are calibration parameters, k_B is the Boltzmann constant and ρ_{eq} is an equilibrium dislocation density (10^{11} m^{-2}). d_{ann} is a critical distance between dislocations for spontaneous annihilation: $d_{ann} = \frac{Gb^4}{2\pi(1-\nu)E_v^f}$, where ν is the Poisson's ratio and E_v^f is a vacancy formation energy. *D* is a self-diffusion coefficient along dislocations: $D = \chi b^2 \nu_D \exp(\frac{-Q}{k_B T})$, where ν_D is the Debye frequency and *Q* is a diffusion activation energy. In order to account for solute atoms we introduce a parameter, χ, which is reverse proportional to the fraction of solute atoms, f_i:

$$\chi = \left(\sum_{\mathrm{i}} \mathrm{f_i^n}\right)^{-\frac{1}{\mathrm{n}}} \tag{2}$$

In Equation(2), *n* is the number of relevant alloy elements. It means that if the fraction of solute atoms increases (e.g. by dissolution of phases), the motion of dislocations and their annihilation is impeded. Thus, a deformed material will be less recovered and this will impact the microstructure development during post-deformation annealing. During the static recrystallization the nucleation of a new grain starts when a growing sub-grain reaches a critical size defined as $\delta_{cr} = \frac{4\gamma_{gb}}{P_D^0 - P_Z}$. Here γ_{gb} is a grain boundary energy, P_D^0 is an initial driving force defined by the dislocation density after deformation and $P_Z = 2\pi\gamma_{gb}N_V r^2$ is a retarding force of nano-size particles (the Zener pinning pressure). Here, N_V is a particle density and *r* is a mean radius calculated by MatCalc. A newly formed recrystallized grain, d_{SRX}, will further grow, if the driving force, P_D, overcomes the retarding force, P_Z: $\frac{dd_{SRX}}{dt} = M_G(P_D - P_Z)$. The grain boundary mobility (M_G) is defined as $M_G = \frac{b^2 D}{k_B T}$. Thus, the grain growth might be also restricted by increasing amount of the solute atoms through the factor, χ. The role of the solute drag has been studied in literature and one of the most recent approaches might be found in (Buken & Kozeschnik, 2017).

By using restart methodology in LS-DYNA®, the deformed material geometry as well as material properties and simulation results, including user-defined results, are passed from one process to the subsequent one. SProC supports this feature by providing the required files and input data for the preparation of the FEM input files. Thus, a closed loop of the data exchange was successfully established and in future, additional parameters could be easily added.

MICROSTRUCTURE EVOLUTION IN A HOT COMPRESSION TEST

A hot compression test performed by a deformation dilatometer (in present work we use DIL 805 A/C of Texas Instruments) is commonly applied to determine the flow curves of a specific alloy at a constant temperature, strain and strain rate. It consists of an initial induction heating process of a specimen and a subsequent deformation step as shown in Figure 3. The cylindrical samples (diameter 5 mm × height 10 mm) were made of a conventional AA2024 alloy with a chemical alloy composition 4.27 wt.% Cu, 1.42 wt.% Mg,

0.4 wt.% Mn, 0.12 wt.% Fe and 0.1 wt.% Si. A typical microstructure of such alloy consists of FCC Al-Matrix, Mg_2Si, θ-Al_2Cu, S-Al_2CuMg, Q-$Al_5Cu_2Mg_8Si_6$ and different Fe-containing intermetallic phases.

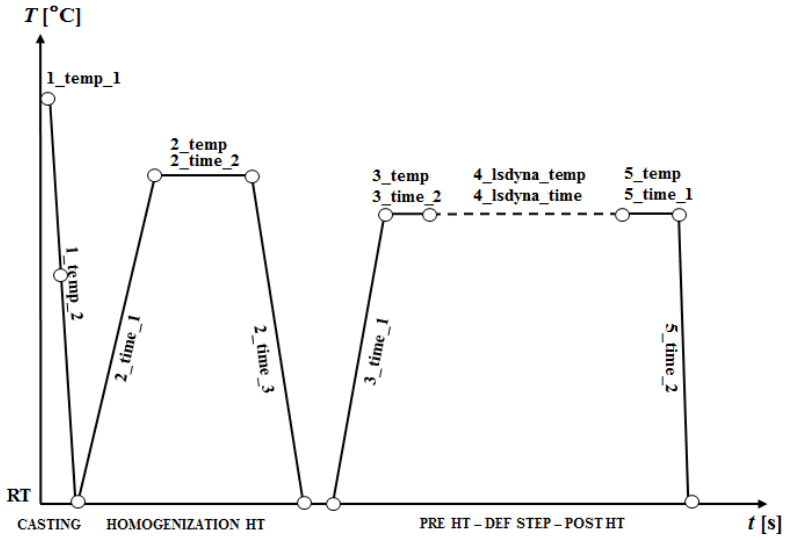

Figure 3. Schematic representation of a simulation sequence.

The deformation test was performed at a constant temperature and strain rate, and the processing parameters are summarized in Table 1. In order to analyze the influence of the precipitation kinetics on development of the material microstructure two tests with different time of iso-thermal heat treatment before deformation were performed. Both samples were annealed for 600 s after the deformation in order to analyze the recrystallization behavior.

Table 1. Deformation processing parameters of a hot compression test.

Process	Parameter	Value
Heating to deformation	Temperature	490 °C
	Heating duration	30 s
	Isothermal holding duration	10 s / 300 s
Deformation step	Mean strain rate	1.0 s^{-1}
	Mean strain	1
Annealing	Time	600 s

As one can see from Figure 4, there is a noticeable decrease in a mean grain size for the samples deformed with longer time of the iso-thermal pre-heat treatment in contrast to samples with shorter time of pre-heat treatment. Thus, it might be supposed that there is a change in microchemistry of the samples during the pre-heating to the deformation temperature which should be analysed.

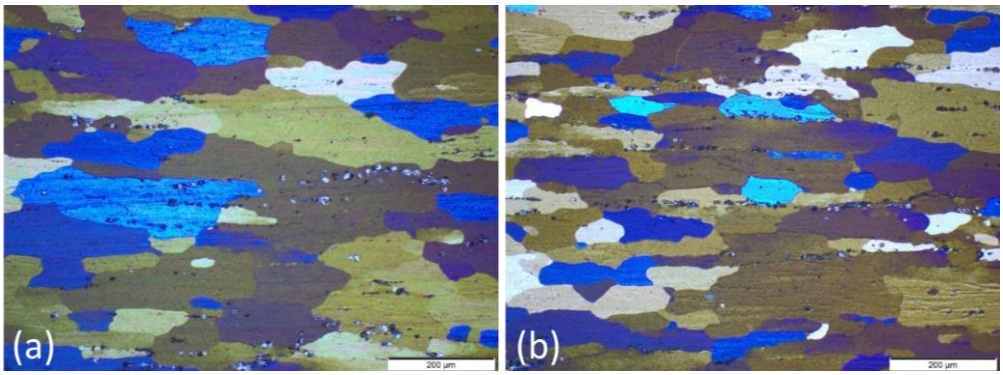

Figure 4. Microstructure of samples deformed at 490°C with (a) 10 s and (b) 300 s of iso-thermal heat treatment before deformation.

RESULTS AND DISCUSSIONS

For modelling of the solidification process and calculation of the primary precipitates, a Scheil-Gulliver approach was used, while for modelling of the precipitation in a solid state, an integrated classical nucleation theory implemented into MatCalc was applied. Based on the chemical alloy composition we have chosen from the thermodynamic database "mc_al_2.030.tdb" the following phases: FCC_A1, S_PHASE, THETA_AL2CU, AL7CU2FE, AL13FE4, Q_PHASE_H, MG2SI_B and ALCUMN_T1. Among them only the ALCUMN_T1 are precipitating as stable nano-size particles (dispersoids) during the homogenization, which are able to retard the recrystallization after the deformation. Due to high dissolution temperature of this phase, almost no significant change of their amount might be expected during pre-heating to a given deformation temperature. However, the experimentally detected Cu/Mg-containing particles might dissolve during the simulation time and this should lead to a noticeable change of the parameter, χ (see Equation (2)), and therefore of the microstructure.

To show the influence of microchemistry on the macroscopic material properties during the deformation, results from identical simulations with the precipitation kinetics calculation during isothermal pre-heat treatment for 10 s and 300 s are compared. The deformation process parameters were in both examples identical. Therefore, the plastic strain and temperature results are identical as well and are given once for both cases in Figure 5. As can be seen in Figure 5 (a) the mean plastic strain of 1 is distributed in a way that maximum values of 1.8 can be found in the specimen center while minimum values near zero can be found at the top and bottom. The maximum temperature can be therefore found in the center of the specimen (Figure 5 (b)) and is 6 °C above the initial temperature.

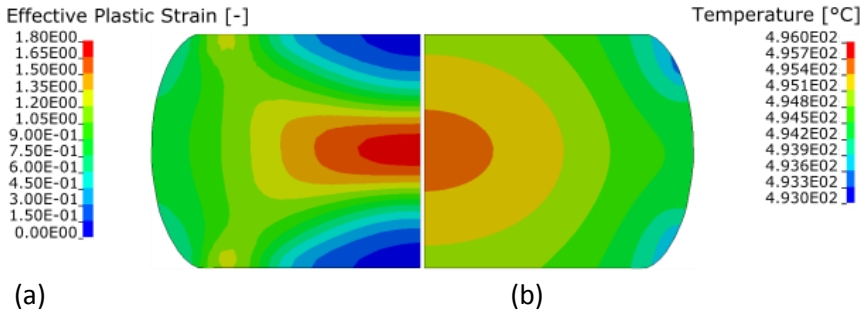

Figure 5. Calculated effective plastic strain (a) and temperature (b) from hot compression test simulations.

Since the plastic strain has a major impact on the evolution of dislocation density, the similarity in the distribution of the dislocation density and plastic strain might be expected (compare 5 (a) and Figure 6).

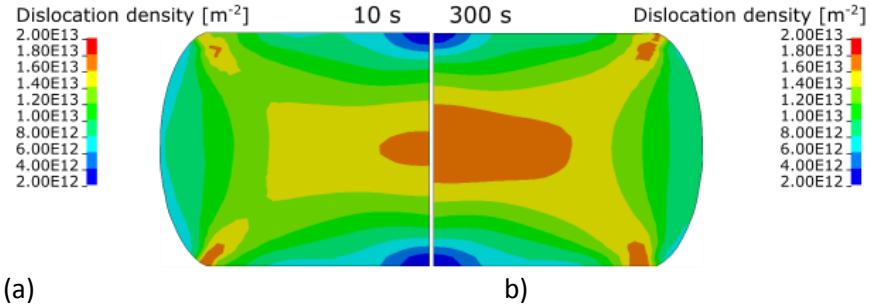

Figure 6. Mean dislocation density results considering simulation of precipitation kinetics after 10 s (a) and 300 s (b) isothermal pre-heat treatment at 490 °C.

One can notice that there a remarkable increase in the dislocation density (ρ_{mean}) with increasing time of the iso-thermal heat treatment before the deformation which can be explained as following. During isothermal heat treatment, the Cu/Mg-containing phases will dissolve leading to decrease of the material parameter, χ, and thus the sample will be less recovered. In other words, the atoms migrating into the Al-matrix act as obstacles for the dislocation motion and increase the materials strength as shown in Figure 7.

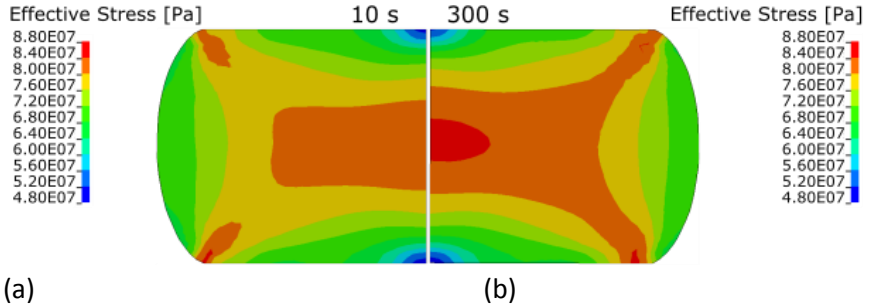

Figure 7. Effective stress results considering simulation of precipitation kinetics after 10 s (a) and 300 s (b) isothermal pre-heat treatment at 490 °C.

By calculation of the static recrystallization during the post-deformation annealing (herein only one-dimensional case based on values from the center of the specimens) a reduction of mean grain size (GS_{mean}) is noticed. While the dislocation density is less recovered, a critical sub-grain size needed to form a new recrystallized grain, δ_{cr}, decreases. At the same time, the grain boundary mobility (grain growth) is pinned by both nano-sized particles and solute atoms. Therefore, a less recrystallized grain fraction and a smaller mean grain size are seen in simulation of samples deformed with a longer time of pre-heating (300 s). The results are summarized in Table 2.

Table 2. Numerically predicted values of material parameters.

Isothermal pre-HT	$\boldsymbol{\chi}$	$\boldsymbol{\rho_{mean}}$ [m^{-2}]	$\boldsymbol{GS_{mean}}$ [µm]
10 s	46	1.6e13	204
300s	41	1.8e13	190

CONCLUSION AND SUMMARY

Incorporating the development of a local microchemistry into the FE simulations of the forming processes is a further step in numerical modelling, and has the potential to improve the product quality and understanding of production issues, e.g. the recrystallization and grain growth. The presented methodology is a first step towards coupling of models for microchemistry (precipitation formation, transformation, dissolution) and microstructure evolution in a framework of the FE solver. Considering the whole production process chain from casting until the forming processes of semi-finished products shows the influence of individual heat treatment steps on the final macroscopic product properties. The given example of the hot compression test clearly shows the influence of microchemistry on the final properties such as a total strength.

The presented implementations are still in an early stage however, they already show the potential of the basic idea. By combining the precipitation kinetics with in-house static recrystallization model implemented into LS-DYNA® material subroutine, the evolution of grain size and recrystallized grain fraction can be calculated during the post-deformation heat treatment in multi-dimensional representation. Furthermore, the coupling with the thermo-kinetic modelling of simultaneous microchemistry evolution during deformation is planned.

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