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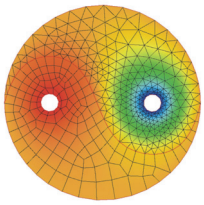

MODELING OF STATIC RECRYSTALLIZATION KINETICS BY COUPLING CRYSTAL PLASTICITY FEM AND MULTIPHASE FIELD CALCULATIONS

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Abstract

In multi-step hot forming processes, static recrystallization (SRX), which occurs in interpass times, influences the microstructure evolution, the flow stress and the final product properties. Static recrystallization is often simply modeled based on Johnson-Mehl-Avrami-Kolmogorov (JMAK) equations which are linked to the visco-plastic flow behavior of the material. Such semi-empirical models are not able to predict the SRX grain microstructure. In this paper, an approach for the simulation of static recrystallization of austenitic grains is presented which is based on the coupling of a crystal plasticity method with a multiphase field approach. The microstructure is modeled by a representative volume element (RVE) of a homogeneous austenitic grain structure with periodic boundary conditions. The grain microstructure is generated via a Voronoi tessellation. The deformation of the RVE, considering the evolution of grain orientations and dislocation density, is calculated using a crystal plasticity finite element (CP-FEM) formulation, whose material parameters have been calibrated using experimental flow curves of the considered 25MoCrS4 steel. The deformed grain structure (dislocation density, orientation) is transferred to the FDM grid used in the multiphase field approach by a dedicated interpolation scheme. In the phase field calculation, driving forces for static recrystallization are calculated based on the mean energy per grain and the curvature of the grain boundaries. A simplified nucleation model at the grain level is used to initiate the recrystallization process. Under these assumptions, it is possible to approximate the SRX kinetics obtained from the stress relaxation test, but the grain morphology predicted by the 2d model still differs from experimental findings.

Key words: static recrystallization, crystal plasticity FEM, multi-phase field method, hot forming, periodic microstructure modeling

1. INTRODUCTION

Microstructural changes play a major role in hot working processes, not only because the microstructure defines force requirements for forming through the flow stress but also since the microstructure defines final product properties. Static recrystallization (SRX) is one of the most dominant mechanisms during inter-pass periods of hot rolling or forging processes and it is a common practice to model its kinetics using Johnson-Mehl-Avrami-Kolmogorov (JMAK) type equations. However, commonly used models such as those proposed by Sellars (1990) lack spatial resolution. They disregard effects of grain topology, misorientations and local accumulations of deformation. Operating on the macro-level, they assume that the microstructure associated with a material point can be described by average values of grain size, dislocation density or even strain. Calculation strategies based on Monte Carlo Potts (Raabe, 1999), cellular automata (Gawad et al., 2008), vertex (Piekos et al., 2008) and multi-phase

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field methods (Takaki & Tomita, 2010) were proposed as an attempt to capture the heterogeneities at the micro level. Among those methods, the phase field method offers a promising approach for modeling static recrystallization after plastic deformation due to its implicit definition of the grain boundaries as a diffusive interface. This simplifies the simulation of interface migration, avoiding the complexity of handling their topology one-by-one. In addition, its theoretical foundation on irreversible thermodynamics allows for the implementation of models based on the minimization of the free energy functional of the polycrystalline microstructure (Steinbach, 2009).

In order to take advantage of the phase field approach in an SRX model effectively, a representative initial (i.e. deformed) state of the microstructure is a necessary starting condition. In recent years, crystal plasticity finite element (CP-FEM) simulations have gained momentum and have now reached a level of high predictive quality. The possibility to implement grain-scale flow stress evolution models and to derive intra- and inter-grain crystalline interactions during deformation enables the generation of a representative deformed microstructure for a phase field simulation (Roters et al., 2010).

However, the results of intricate models with spatial resolution are often not compared to experimental results. In this paper, the microstructural evolution of a commercial steel grade (25MoCrS4) during SRX after a hot uniaxial compression test is simulated by coupling CP-FEM calculations and phase field simulations. A 2d microstructure is generated via a Voronoi algorithm, used to set up a CP-FEM model with random grain orientations, and subjected to uniaxial compression. The results of CP-FEM simulation are mapped onto the finite difference grid of the multi-phase field SRX simulation. Finally, predicted values are critically compared with the results of stress relaxation test.

2. EXPERIMENTAL ANALYSIS

2.1. Material

The steel grade 25MoCrS4, a case hardening steel for gearing applications for automotive and aerospace industry, was selected as application material. Its chemical composition is given in Table 1.

2.2. Compression tests

The hardening response of the material was obtained through a set of compression tests at 1100°C and at five different strain rates: $\dot{\varphi}$ = 0.01, 0.1, 1, 10 100 s^{-1}. Exact procedures of sample preparation and experimental methodology are described elsewhere (Henke et al., 2011). Fig. 1 shows deformation response of the material under uniaxial compression at 1100°C.

2.3. Stress relaxation tests

The SRX kinetics of the material were examined by stress relaxation tests. The compression test specimens (without lubrication pockets) were deformed to a pre-strain below the critical strain for dynamic recrystallization (DRX) at the different strain rates. After the predefined strain level was reached, the cross-head of the servo-hydraulic testing machine was kept at constant height and the force response of the specimen was measured over time. The decrease of the reaction force and the respective stress values were then converted to recrystallized volume fractions (X_{RX}) according to the procedure described by (Gronostajski et al., 1983). Once the time evolution of X_{RX} is known, JMAK kinetics of SRX can be evaluated by determining the unknown parameters of the modified Avrami equation:

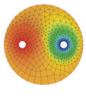
$$X_{RX} = 1 - \exp\left[-\ln 2\left(\frac{t}{t_{0.5}}\right)^{n}\right], \qquad (1)$$

in which n is the Avrami exponent and $t_{0.5}$ denotes the time required to reach 50% recrystallization. For the given values of $X_{RX}(t)$ and $t_{0.5}$, an Avrami exponent of n = 0.56 was determined by regression for the test case strain: φ = 0.2, strain rate: $\dot{\varphi}$ = 0.01 s^{-1} at T = 1100°C.

Light optical microscopy (LOM) was used before and after SRX in order to determine the grain size evolution and nucleation site preference. For details of the sample preparation we refer to Xiong et al. (2011). LOM results show that the average grain sizes before and after the SRX are ~36 µm and ~7 µm, respectively, for all considered strain rates.

Table 1. Chemical composition of 25MoCrS4 (1.7326) according to DIN 17210 (Values are in wt. %).

Grade	C	Mn	Si	Cr	Mo
25MoCrS4	0.23 – 0.29	0.60 – 0.90	0.15 – 0.40	0.40 – 0.50	0.40 – 0.50



In addition, nucleation sites of the SRX are not found inside the grains, but on the grain boundaries.

3. MICROSTRUCTURE MODEL

3.1. Deformation model

In order to simulate the plastic hardening behavior, the well-known phenomenological deformation law by Hutchinson (1976) is used within the simulation software DAMASK (Roters et al., 2012). The law is defined by

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left| \frac{\tau^{\alpha}}{\tau_c^{\alpha}} \right|^{\frac{1}{m}} sgn\left(\tau^{\alpha}\right), \tag{2}$$

$$\dot{\tau}_c^{\alpha} = \sum_{\beta=1}^{n} h_{\alpha\beta} \left| \dot{\gamma}^{\beta} \right|, \tag{3}$$

where α denotes the active slip system, $\dot{\gamma}^{\alpha}$ is the shear rate at the active slip system, $\dot{\gamma}_0$ is any convenient reference shear rate, τ^{α} and τ_c^{α} denote the stress state and the critical resolved shear stress on the active slip system, m characterizes the strain rate sensitivity and finally $h_{\alpha\beta}$ is the function defining the incremental value of τ_c^{α} in terms of shear increments on a chosen slip system β, which can be calculated using the equation

$$h_{\alpha\beta} = h_0 \left(1 - \frac{\tau_c^{\alpha}}{\tau_{sat}}\right)^{a}, \tag{4}$$

In equation (4), h_0, a and τ_{sat} are material parameters (Kalidindi et al., 1992). The parameter set can be calibrated with the compression test results.

The macro-scale stress-strain curve can be converted to its micro-scale counterpart by the method proposed by Taylor (1938). If the material is assumed to be isotropic throughout the deformation process (i.e. Taylor factor M = 3), initial and saturation values of the slip resistance can be determined (τ_0 = 8 MPa, τ_{sat} = 16 MPa) and the other model parameters can be calculated numerically (h_0 = 300 MPa, a = 2). Fig. 1 shows the comparison of experimental and numerical responses of the material. Note that each experiment has been repeated five times in order to take the experimental scatter into account.

3.2. Coupling

Three types of data have to be mapped from the CP-FEM output to the phase field simulation: The grain index, the mean grain orientation and the mean stored energy per grain. However, the transfer of data from a FEM mesh to a FDM grid requires a dedicated interpolation scheme. In order to transfer the grain index and the grain orientation data from nodes to the grid, it is assumed that each grid point has the index and orientation value of its nearest neighboring node as shown in Fig. 2.

In addition, the local orientations have to be averaged after the mapping to determine the mean grain orientations using circular statistics (Berens, 2009). The stored energy of the deformation can be calculated from the flow stress increase using the equations

$$\tau_c = \tau_0 + \alpha G b \sqrt{\rho}\,, \tag{5}$$

$$E_d = \alpha \rho G b^2\,, \tag{6}$$

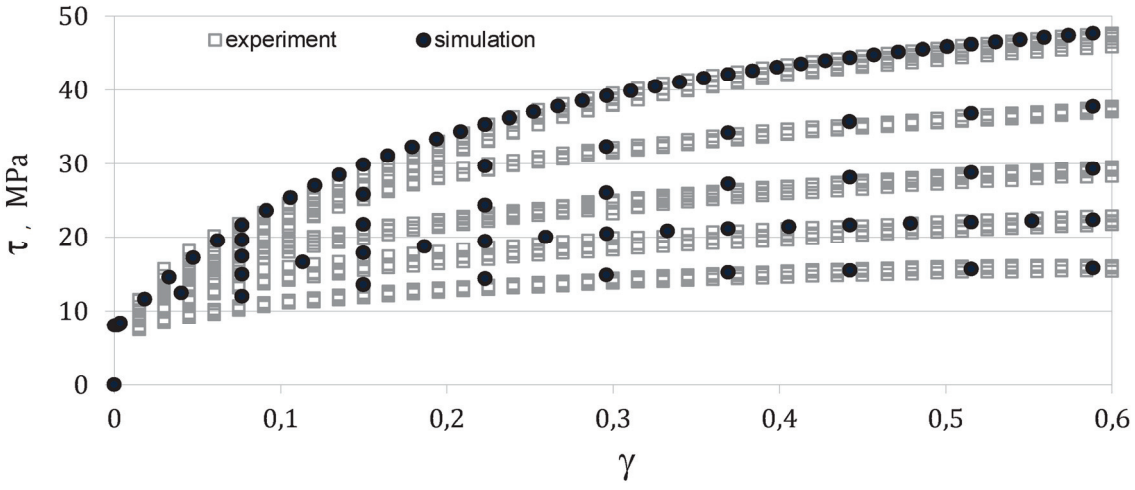


Fig. 1. *Comparison of CPFEM and compression test results of 25MoCrS4 at 1100°C at various strain rates.*

$$E_d = \frac{(\tau_c - \tau_0)^2}{\alpha G}. \qquad (7)$$

In the equations (5), (6) and (7), E_d is the stored energy due to deformation, α defines a proportionality constant, $G(T)$ is the temperature dependent shear modulus, τ_c and τ_0 are the final and initial values of the shear resistance (Taylor, 1934). Then, the nodal energies are mapped onto the grid points.

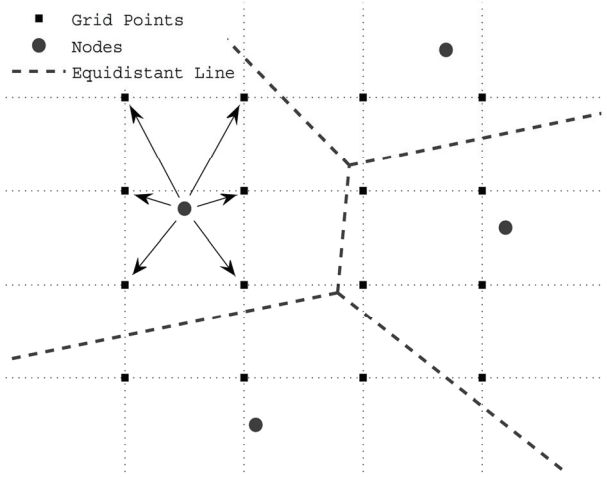


Fig. 2. *The index and orientation of a node(circle) is assigned to all grid points (square) which are far away from the other nodes.*

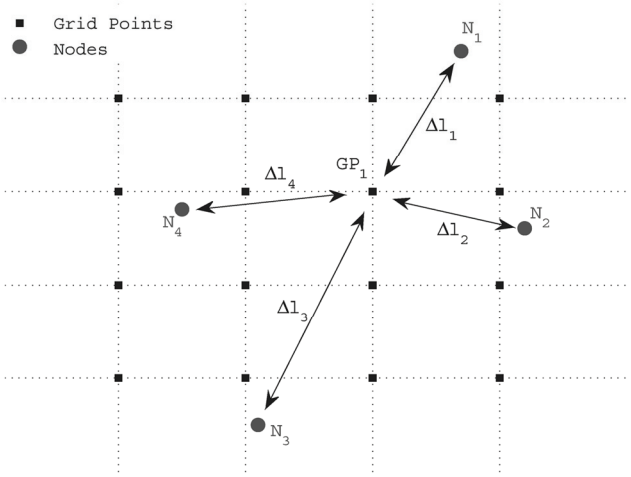


Fig. 3. *The energy E_d of each grid point (GP) is determined by interpolating that of the nodes. Influence of each node is inversely proportional to its distance to an individual GP.*

In the mapping, the interpolated values at the gird points are obtained as the weighted sum of adjacent finite element mesh nodes. The weights are inversely proportional to the relative distance between grid point and finite element node, as illustrated in Fig. 3.

Finally, the mean stored energy per grain is found by calculating their arithmetic mean on the grain area. Note that, at the moment no dislocation density gradients inside the grains are taken into account.

3.3. Recrystallization model

For an isothermal, heterogeneous system, grain evolution can be modeled by minimization of the free energy functional – under the assumption of a double obstacle function – which leads to the popular formulation of multi-phase field method, expressed via equation (8) (Eiken et al., 2006).

$$\phi_i = \sum_j m_{ij}\Big[\sigma_{ij}\underbrace{\Big(\phi_i\nabla^2\phi_j - \phi_j\nabla^2\phi_i + \frac{\pi^2}{2\eta^2}\big(\phi_i - \phi_j\big)\Big)}_{\kappa_{ij}} + \frac{\pi}{\eta}\sqrt{\phi_i\phi_j}\,\Delta G_{ij}\Big] \qquad (8)$$

In equation (8), η is the interface thickness, m_{ij} is the grain boundary mobility, σ_{ij} denotes the interfacial energy between adjacent grain boundaries, κ_{ij} is related to the grain boundary curvature and ΔG_{ij} is the contribution of the stored energy (E_d). Therefore, equation (8) models the combined effects of curvature and stored energy on the interface migration. In addition, the nucleation of new grains was assumed to take place at interfaces and triple junctions with site saturation as initial condition.

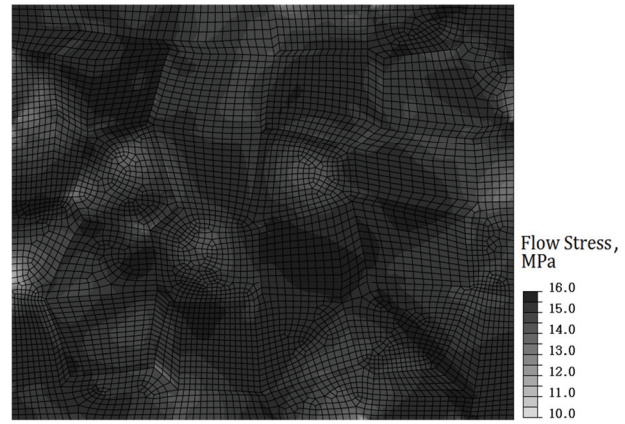
4. SIMULATION AND RESULTS

4.1. Deformation

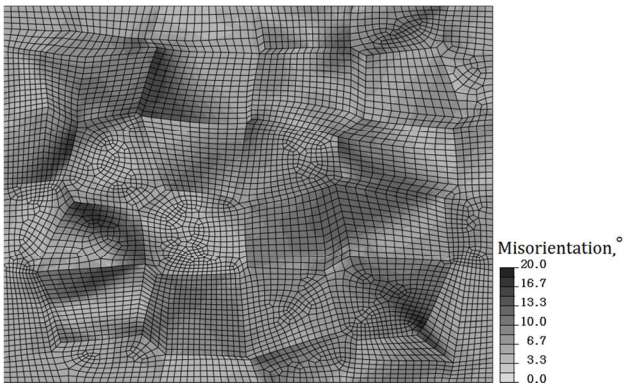
Isothermal uniaxial compression at a constant strain rate (T = 1100°C and $\dot{\varphi}$ = 0.01 s^{-1}) under homogenous boundary conditions was simulated with periodic digital microstructure generated by a planar Voronoi tessellation of 25 randomly oriented grains. In order to avoid the occurrence of DRX, a maximum strain of 0.2 was imposed in the stress relaxation experiments, and the same pre-strain was used in the model. Evolution of slip resistance and misorientation are shown in Fig. 4.

4.2. Recrystallization

After the deformation simulation, the local stored energies were converted to mean energies per grain using equation (7) with G = 32.2 GPa and α = 0.54 and converted to the FDM grid. In the SRX simulation η was taken to be 1.5 μm, the surface



a)



b)

Fig. 4. *(a) τ_c and (b) misorientation at the end of deformation.*

energy was set to 3e-7 Jcm^{-2} and the mobility was assumed to be 5e-3 cm^4/Js. Nucleation was restricted to occur at the grain boundary interfaces and at triple junctions and only at sites where the stored energy exceeds 2.5e-2 Jcm^{-3}. When these values are chosen, the SRX kinetics and grain sizes of the phase field simulation are in good correlation with the experimental values as seen in Fig. 5 and Table 2. However, the Avrami exponent calculated from the phase field model is observed to be larger than 1 in contrast to the exponent from the experiment.

The evolution of the morphology of the deformed microstructure during the SRX was also predicted. It was found that with the aforementioned parameter set, the recrystallized grain front is directional which results in a cuboidal final microstructure as shown in Fig. 6.

Table 2. *Comparison of mean grain sizes calculated by LOM and CPFEM-PF after recrystallization*

Mean grain diameter / µm	LOM	CPFEM-PF
After recrystallization	7	8.2

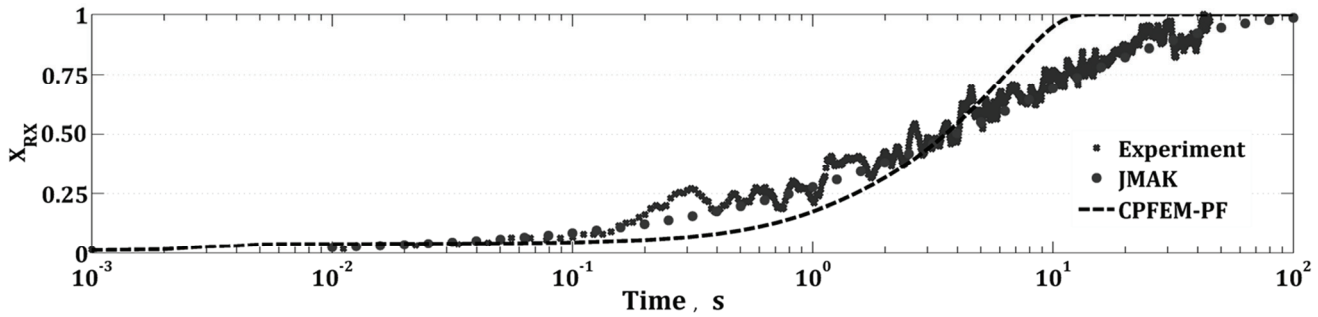


Fig. 5. *X_{RX} kinetics of CPFEM-PF-simulation, JMAK model and the stress relaxation experiment.*

(a) t = 0.1 s **(b) t = 1 s** **(c) t = 100 s**

Fig. 6. *Progression of recrystallization through time: (a) Growth of nuclei on the interfaces, (b) their competitive growth towards non-recrystallized grains and (c) the fully recrystallized microstructure.*

5. DISCUSSION

5.1. CP-FEM and coupling

The microstructural deformation of 25MoCrS4 is successfully modeled by CPFEM using a well-established phenomenological hardening law. Material parameters are calibrated using the experimental results at the macro-scale. Even though the model is phenomenological, the inter-/intra-grain scatter of the grain orientation and hardening are captured and mapped onto finite difference grid effectively. However, due to the usage of the mean orientation and stored energy per grain in the phase field simulation, the scatter is unintentionally averaged during mapping which results in a loss of resolution. This problem can be solved in the future by accounting for dislocation gradients and abnormal sub-grain growth in order to improve the simple nucleation model at the grain level.

5.2. Static recrystallization

The SRX kinetics and grain size calculated with the phase field method show a good correlation with that of the stress relaxation experiments. The morphological evolution of the microstructure is found to be directional, resulting in unrealistic cuboidal final grain geometry. Due to the low experimental value of the Avrami exponent ($n < 1$), it was necessary in this model to fill all possible nucleation sites. The usage of a 2D model and the assumption of site saturation restrict the number of nucleation sites (i.e. number of sites per interface) that is available. An extension to 3D space would increase the number of possible nucleation sites per interface and make the predicted grain morphology more realistic.

6. CONCLUSION

In this work a coupled CP-FEM-phase field model based on the mean stored deformation energy and grain boundary curvature is applied to predict SRX kinetics. This mean energy per grain serves as driving force in the recrystallization simulation with the multi-phase field approach. In contrast to conventional JMAK based statistical models, the applied model comprises only physical quantities, e.g. surface energy and interfacial mobility which allow for physical interpretation. Moreover, being a spatially resolved method, the phase field method takes the heterogeneity of the stored energy and boundary curvature into account.

A dedicated mapping scheme was used to couple the multi-phase field model with a CPFEM deformation model whose deformation conditions correspond to experimental results. The mapping algorithm averages out local gradients and should be improved in the future. The nucleation mechanism of the 2-D model leads to a rather unrealistic grain shape when the model is adjusted to the experimentally obtained SRX kinetics. In spite of the good correlation between model and experiment, a 3-D model with an improved nucleation model at the grain level is necessary to predict the SRX kinetics and the final grain shape more accurately.

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MODELOWANIE KINETYKI REKRYSTALIZACJI STATYCZNEJ POPRZEZ SPRZĘŻENIE PLASTYCZNOŚCI KRYSZTAŁÓW MES Z OBLICZENIAMI PÓL WIELOFAZOWYCH

Streszczenie

W wielostopniowych procesach obróbki plastycznej, rekrystalizacja statyczna (ang. static recrystallization - SRX) występująca w czasach przerw między odkształceniami, wpływa na rozwój mikrostruktury, naprężenie uplastyczniające oraz właściwości gotowego produktu. Statyczna rekrystalizacja jest często modelowana korzystając z równania Johnson-Mehl-Avrami-Kolmogorov (JMAK), które jest powiązane z lepkoplastycznym płynięciem materiału. Taki pół-empiryczny model nie jest w stanie przewidzieć mikrostruktury ziaren dla SRX. W niniejszym artykule przedstawiono podejście do symulacji statycznej rekrystalizacji austenitu wykorzystujące połączenie plastyczności kryształów z metodą pola wielofazowego. Mikrostruktura jest modelowana za pomocą reprezentatywnych elementów objętości (ang: Representative Volume Element - RVE) jednorodnej struktury ziaren austenitu z okresowymi warunkami brzegowymi. Mikrostruktura jest generowana za pomocą wieloboków Voronoi. Obliczenia odkształcenia RVE są prowadzone połączonymi metodami plastyczności kryształów i MES, z uwzględnieniem rozwoju orientacji ziaren oraz gęstości dyslokacji. Parametry modelu materiału wyznaczono na podstawie doświadczalnych krzywych płynięcia dla stali 25MoCrS4. Odkształcona struktura ziaren (gęstość dyslokacji, orientacja) jest przekazywana do siatki różnic skończonych w modelu pola wielofazowego stosując metodę interpolacji. W obliczeniach pola faz, siły pędne dla statycznej rekrystalizacji są obliczane na podstawie średniej energii w ziarnie i krzywizny granic ziaren. W celu zainicjowania rekrystalizacji stosowany jest uproszczony model zarodkowania na poziomie ziarna. Przy tych założeniach możliwe było oszacowanie kinetyki SRX na podstawie badań relaksacji naprężeń. Z drugiej strony przewidywana w modelu 2D morfologia ziaren wciąż odbiega od wyników doświadczalnych.

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