MICROSTRUCTURE EVOLUTION SUBROUTINE FOR FINITE ELEMENT ANALYSIS

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ABSTRACT

Existing Finite Element Method software can be used in a broad field of material characterization, such as heat conduction, plasticity, electric conductivity or fluid mechanics. However, in terms of microstructure, there is a lack of sophisticated packages to thoroughly model the evolution of these parameters. In the present work, a simple but extensive subroutine is presented, to express the kinetics of precipitation and grain growth on the one hand, and the evolution of structural defects, such as dislocation density and vacancy concentration, on the other hand, in dependence of temperature and deformation rate. As a result, further technologically important material properties, such as yield strength, can be derived with the knowledge of aforementioned parameters. The basic functionality of the subroutine is outlined and the handling of the state parameters, which are used during calculation, are explicated.

Keywords: microstructure evolution, strengthening

INTRODUCTION

In the field of manufacturing, it is crucial to understand residual stress and distortions that may occur during production. This helps in optimizing both, component design and processing parameters. The complete manufacturing process, starting from solidification, must be considered to simulate stress evolution that depends on temperature and strain rate. An accurate material model is necessary to link flow stress to plastic strain, and various models have been developed over the years [1-5]. Nowadays, empirical models or data table methods are standard and integrated into most Finite Element (FE) software tools such as ANSYS or ABAQUS.

The present work is based on the "simple MicroStructure Evolution" (sMSE) model, which has been introduced by Viernstein et al. [6], in which the treatment of the yield strength and precipitates is thoroughly described. The current work can be seen as a supplement for the aforementioned work. Instead of focusing on strengthening mechanisms, the structure of the subroutine is rolled up from a microstructural point of view. The focus will be on lattice defects, namely point defects (vacancies), line defects (dislocations), planar defects (grain boundaries) and bulk defects (precipitates). A short

overview is also given of all defect evolution equations with particular emphasis on their interdependence. A brief overview on the usage of the subroutine is presented as well.

MICROSTRUCTURE EVOLUTION

VACANCIES

The evolution of the vacancy concentration, X_{Va}, is described using the FSAK framework introduced by Fischer et al. [7]. Vacancies can form and annihilate at dislocation jogs

$$\Delta X_{\mathrm{Va,d}} = -\frac{X_{\mathrm{Va}}}{X_{\mathrm{Va,eq}}}\frac{D_{\mathrm{m}}}{f}2\pi\rho X_{\mathrm{j,eq}}\log\left(\frac{X_{\mathrm{Va}}}{X_{\mathrm{Va,eq}}}\right), \tag{1}$$

and grain boundaries

$$\Delta X_{\mathrm{Va,gb}} = -\frac{X_{\mathrm{Va}}}{X_{\mathrm{Va,eq}}}\frac{D_{\mathrm{m}}}{f}15\pi\frac{1}{R^2}\log\left(\frac{X_{\mathrm{Va}}}{X_{\mathrm{Va,eq}}}\right), \tag{2}$$

where $X_{\mathrm{Va,eq}}$ is the equilibrium vacancy concentration, D_{m} the effective matrix diffusion coefficient, f a geometrical correlation factor (0.7815 for fcc and 0.7272 for bcc), ρ the dislocation density, $X_{\mathrm{j,eq}}$ the jog fraction at equilibrium (estimated to be around 0.02) and R the grain radius.

Excess vacancies form during quenching and can accelerate the effective matrix diffusion of elements, D_{eff}, by several orders of magnitude until their annihilation

$$D_{\mathrm{eff}} = D_m\frac{X_{\mathrm{Va}}}{X_{\mathrm{Va,eq}}}. \tag{3}$$

The vacancy concentration has no direct influence on the evaluation of stresses. However, it has a severe influence on all long-range diffusion processes, especially precipitation kinetics.

DISLOCATIONS

The evolution of the dislocation density ρ is described by a simple modified Kocks and Mecking model [8]

$$\Delta\rho = \frac{M}{bA}\sqrt{\rho}\dot{\varepsilon} - 2BM\frac{d_{\mathrm{crit}}}{b}\rho\dot{\varepsilon} - 2CD_d\frac{Gb^3}{k_{\mathrm{B}}T}\left(\rho^2 - \rho_{\mathrm{eq}}^2\right), \tag{4}$$

where M is the Taylor factor, $\dot{\varepsilon}$ the strain rate, b the Burger's vector, d_{crit} the critical annihilation distance between dislocations, D_d the diffusion coefficient along dislocations, G the shear modulus, k_{B} the Boltzmann constant, ρ_{eq} the equilibrium dislocation density and A, B and C material parameters. These material parameters can be either defined as user input or calculated with the initial hardening rate θ and the saturation stress σ according to the model introduced by Kreyca et al. [9].

The dislocation density contribution to the stress is evaluated by the Taylor equation [10]

$$\sigma_{\mathrm{d}} = \alpha M b G \sqrt{\rho}, \tag{5}$$

with α being the dislocation strengthening coefficient. Furthermore, dislocations act as sources and sinks for vacancies, as mentioned above, or can be seen as possible nucleation sites for precipitates.

GRAIN BOUNDARIES

Grain boundaries are described by the average grain radius R and their evolution by the formula for ideal grain growth [11]

$$\Delta R = 2 k_{\mathrm{D}} M \frac{\gamma}{R}, \tag{6}$$

where k_{D} is the proportionality factor, M the mobility of the grain boundary and γ the grain boundary energy. Their contribution to the stress is described by the Hall-Petch equation for fine grain hardening [12,13]

$$\sigma_{\mathrm{FG}} = \frac{K}{\sqrt{2R}}, \tag{7}$$

where K is the Hall-Petch coefficient.

The evolution of the grain radius is, like the dislocation density, not dependent on other defect types (in the current version of the subroutine, pinning of grain boundaries by precipitates is not yet considered). However, they influence the generation and annihilation of vacancies and can act as potential nucleation sites for precipitates.

PRECIPITATES

The kinetics of precipitation and their influence on stress is described in detail in the original work of Viernstein et al. [6]. Here, a short summary of the key aspects and an emphasis on the interdependence with the other defect types is presented. The nucleation rate of precipitates, J, is given by classical nucleation theory [14]

$$J = N_0 Z \beta e^{-\frac{G^*}{k_{\mathrm{B}} T}}, \tag{8}$$

where N_0 is the number of available nucleation sites, Z the Zeldovich factor, β the atomic attachment rate and G^* the critical nucleation energy. N_0 is calculated depending on the type of nucleation site

$$N_{0,\mathrm{d}} = P_{\mathrm{d}} \frac{\rho}{b}, \tag{9}$$

$$N_{0,\mathrm{gb}} = P_{\mathrm{gb}} \frac{An}{b^2}, \tag{10}$$

where P_{d} and P_{gb} are the efficiencies of dislocation and, respectively, grain boundary nucleation sites, ρ the dislocation density, b the Burger's vector, A the area of one grain

and n the number of grains per unit volume. The atomic attachment rate is proportional to the effective diffusion coefficient in the matrix and, therefore, influenced by the vacancy concentration. As a result, a higher supersaturation of vacancies leads to a faster precipitate nucleation process.

The growth of precipitates is described by the original SFFK growth by Svoboda et al. [15]

$$\Delta r = \frac{d}{k_B T}\frac{1}{r} D_{\text{eff}}, \tag{11}$$

where d is the driving force. Similar to the nucleation process, the growth is also directly affected by the vacancies.

SUBROUTINE

The subroutine is written in C code and consists of a single function 'myuserfunc_' taking 9 arguments, which are described in Table 1. During the FE simulation, all relevant variables are saved in the state variable vector (see Table 2 for the structure), which consists of 222 lines. The subroutine covers 4 modes of execution, which can be set by the call mode. The first call mode (1) initializes the material parameters in the state variable vector based on the default settings and should be run once before the FE calculation. An initialization from external is also possible with call mode (2). The main call mode (3) is used for the iteration process during the FE simulation. The subroutine evaluates the evolution of the current state variables (lines 123 to 170 in the state vector) for the given timestep, temperature, and strain rate and saves it without overwriting the current state variables (lines 171-218). The first state variable is the time and is always compared to the calculated time from the last iteration. If the current time (line 123) is set to the calculated time (line 171), the last iteration process is counted as accepted and the calculated state variables will be transferred into the lines of the current ones. The last call mode (4) is reserved for the final call and writes the results of the evaluated stress and its derivatives into the output variables.

Table 1 Arguments for SMSE subroutine

argument	C type	I/O	description
piCallMode	int*	input	call mode of subroutine (1-4)
pdTimeIncrement	double*	input	time increment for current iteration
pdTemp	double*	input	temperature
pdTempIncrement	double*	input	temperature increment for current iteration
pdStrainRate	double*	input	strain rate
vStateVec	double[222]	input/output	state variable vector
pdSigma	double*	output	evaluated stress
pdJacStrain	double*	output	derivative of evaluated stress according to temperature
pdJacStrain	double*	output	derivative of evaluated stress according to strain rate

Table 2 Structure of the state variable vector 'vStateVec'

index	variables	I/O	description
0-38	material parameter	input	basic material properties
39-66	material parameter	input	dislocation evolution
67-71	material parameter	input	solid solution strengthening
72-82	material parameter	input	cross core diffusion
83-118	material parameter	input	precipitate evolution
119-122	material parameter	input	vacancy evolution
123-170	state variable	input	state variables at beginning of current time step
171-218	state variable	output	calculated state variables for time step
219-221	numerical parameter	input	switches for numerical methods

SUMMARY

A compendium of formulas describing the evolution of lattice defects, such as vacancies (point defects), dislocations (line defects), grain boundaries (planar defects) as well as precipitates (bulk defects) during thermo mechanical treatments is presented. While the dislocation density evolution is mainly dependent on the strain rate, grain growth follows from material properties. The vacancy evolution follows from the dislocation density and grain size. Precipitation kinetics is finally derived by the former parameters. The focus is laid on efficient processing for computationally demanding calculations without losing the interdependence of microstructural properties and their influence on the mechanical properties of the material.

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References

[1] P. LUDWIK: 'Über den Einfluss der Deformationsgeschwindigkeit bei bleibenden Deformationen mit besonderer Berücksichtigung der Nachwirkungserscheinungen', *Phys. Zeitschrift*, Nr. 12, pp. 411-417, 1909.

[2] E. VOCE: 'A Practical Strain Hardening Function', *Metallurgia*, pp. 219-226, 1955.

[3] G.R. JOHNSON, W.H. COOK: 'A Constitutive Model and Data for Metals Subjected to Large Strains, High Strain Rates and High Temperatures', *Proc. Seventh Int. Symp. Ballist.*, pp. 541-547, 1983.

[4] F.J. ZERILLI, R.W. ARMSTRONG: 'Dislocation-Mechanics-Based Constitutive Relations for Material Dynamics Calculations', *J. Appl. Phys*, Vol. 61, pp. 1816-1825, 1987.
[5] S. HUANG, A.S. KHAN, S. HUANG, A.S. KHAN: 'Modelling the Mechanical Behavior of 1100-0 Aluminum at Different Strain Rates by the Bodner-Partom Model', *Int. J. Plast.*, Vol. 8, pp. 501-507, 1992.
[6] B. VIERNSTEIN, T. WOJCIK, E. KOZESCHNIK: 'State Parameter-Based Yield Strength Model for Integration in Finite Element User-Material Routines', *Metals*, Vol. 12, No. 1207, pp. 1-16, 2022.
[7] F.D. FISCHER, J. SVOBODA, F. APPEL, E. KOZESCHNIK: 'Modeling of Excess Vacancy Annihilation at Different Types of Sinks', *Acta Mat.*, Vol. 59, pp. 3463-3472, 2011.
[8] P. SHERSTNEV, P. LANG, E. KOZESCHNIK: 'Treatment of Simultaneous Deformation and Solid-State Precipitation in Thermo-Kinetic Calculations', *ECCOMAS 2012 – Eur. Congr. Comput. Methods Appl. Sci. Eng. E-b. Full Pap.*, No. Eccomas, pp. 5331-5338, 2012.
[9] J. KREYCA, E. KOZESCHNIK: 'State Parameter-Based Constitutive Modelling of Stress Strain Curves in Al-Mg Solid Solutions', *Int. J. Plast.*, Vol. 103, pp. 67-80, 2018.
[10] G.I. TAYLOR: 'The Mechanism of Plastic Deformation of Crystals Part I - Theoretical', *Proc. R. Soc. A Math. Phys. Eng. Sci.*, Vol. 145, pp. 362-387, 1934.
[11] G. GOTTSTEIN: *Materialwissenschaft und Werkstofftechnik Physikalische Grundlagen*, Berlin, pp. 361ff, 2014.
[12] E.O. HALL: 'The Deformation and Ageing of Mild Steel: III Discussion of Results', *Proc. Phys. Soc. Lond.*, Vol. 64, No. 9, pp. 747-753, 1951.
[13] N.J. PETCH: 'The Cleavage Strength of Polycrystals', *J. Iron Steel Inst. London*, Vol. 173, pp. 25-28, 1953.
[14] K.C. RUSSELL: 'Nucleation in Solids: The Induction and Steady State Effects', *Adv. Colloid Interface Sci.*, Vol. 13, pp. 205-318, 1980.
[15] J. SVOBODA, F.D. FISCHER, P. FRATZL, E. KOZESCHNIK: 'Modelling of Kinetics in Multi-Component Multi-Phase Systems with Spherical Precipitates I: Theory', *Mater. Sci. Eng. A*, Vol. 385, pp. 166-174, 2004.