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Multiscale modeling of tempering of AISI H13 hot-work tool steel – Part 2: Coupling predicted mechanical properties with FEM simulations

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ABSTRACT

Simulation of austenitization and quenching of steel using the Finite Element Method (FEM) is nowadays a common tool to predict residual stresses and deformations during these processes. However the simulation of tempering, which determines the final residual stresses and distortions has been often neglected or performed in a purely phenomenological and highly simplified way. The objective of this study is to precisely predict the relaxation of internal stresses during tempering, taking explicitly into account the evolution of the microstructure. Mechanical properties which determine the relaxation of stress; namely the drop of the yield stress and the creep mechanism are the key factors for the success of the simulation. These mechanical parameters can be determined experimentally for a specific tempering temperature. However tempering temperature for most steels varies for each industrial application in order to adjust the desired hardness–toughness relation. Consequently, experimentally measurement of decisive mechanical properties which determine the amount of stress relaxation for each tempering temperature is very costly. Therefore, these material parameters were simulated from physically based material models with coupled microstructural simulations in the first part of this two-part investigation. In this part of the study, the simulated mechanical properties will be coupled with the FEM simulations using "Abaqus®", in order to simulate the stress relaxation during the tempering process of a thick-walled workpiece made of hot-work tool steel AISI H13 (DIN 1.2344, X40CrMoV5-1). Utilizing this methodology, different tempering conditions (soaking time, tempering temperature) can be considered in the model to predict the stress relaxation in macroscopic scale.

1. Introduction

FEM simulation of the heat treatment of steels is becoming an important tool for a better estimation of the microstructure, hardness, strength, residual stress and deformation of the workpiece. Several studies concentrate on the simulation of austenitization and the quenching process. [1–6]. On the other hand, although the development of the microstructure during tempering is well known for many steels, only a few FEM studies of the tempering process considering phase transformations and phase dependent material properties exist in the literature [7–15].

Although existing thermo-mechanical–metallurgical models to calculate the relaxation of residual stresses and distortions during tempering consider various effects (phase transformations, drop of yield stress, creep, etc.), the prediction accuracy is still poor [8,10]. Moreover these models require several material parameters which can be determined only from very costly experiments, which are only valid for a specific tempering condition (soaking time, temperature).

In this work, simulation of the whole heat treatment cycle of a thick-walled hot-work tool steel AISI H13 workpiece was established using a thermo-mechanical–metallurgical model. The last step of the simulation cycle namely tempering was conducted with mechanical properties determined experimentally and computationally (see the first part of this study) for the tempering temperatures 600 and 650 °C. Simulated residual stresses were verified against experimental findings. The differences of the calculated residual stresses between simulations with experimental and simulated material parameters will be compared and the possible error potential will be discussed.

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2. Material modeling and numerical implementation in Abaqus®

Coupling of the thermal, metallurgical and mechanical phenomena to describe the heat treatment process was first established by Inoue et al. with the so called metallo-thermo-mechanical model [9,16–21]. The model used here is based on the model of Inoue et al. and considers these three distinct physical fields: (1) thermal, (2) metallurgical and (3) mechanical effects and the important couplings between them. In Fig. 1, solid arrows represent coupling terms which are considered in this model, whereas, dotted arrows represent weak couplings which are currently neglected.

In the literature, there are several implementations of metallo-thermo-mechanical model in Abaqus® by using the so called "UMAT" (user defined material) subroutine [2,22–25]. The most important disadvantage of using "UMAT" is the necessity of defining the Jacobian matrix. Considering the complex constitutive equation (Eq. (8)) of heat treatment, deriving the exact "consistent tangent modulus" is a challenging task. Furthermore, even minor modifications in constitutive equations may require derivation of the tangent once more. Consequently in this study, several other user defined subroutines (UHARD, UEXPAN, UFIELD, HETVAL, etc.) are coupled in order to implement the metallo-thermo-mechanical interactions during heat treatment. Utilizing this methodology, there is no need to define the Jacobian matrix by the user.

2.1. Modeling the heat transfer

The transient heat transfer during heat treatment can be described mathematically by a suitable form of Fourier's heat conduction equation by considering that the thermal field is also altered by the latent heat of phase transformations:

$$\rho c_p \dot{T} = \nabla \cdot (\nabla(\lambda T)) + \dot{Q} \tag{1}$$

where ρ density, c_p specific heat and λ thermal conductivity of the phase mixture and $\dot{Q}$ is the internal heat source due to latent heat. Considering heat treatment simulation of steel, necessary modifications in this equation are the description of the phase and temperature dependent thermal material properties and the heat generation due to phase transformations ($\dot{Q}$).

In this work, thermal properties of the phase mixture were calculated by using the linear rule of mixture. "USDFLD" (user defined field) subroutine in Abaqus® was used to define material properties as a function of "field variables". "Field variables" can be defined in the subroutine "USDFLD" as a solution dependent parameter and can be accessed in the input file of Abaqus®. For the purpose of simulation of heat treatment field variables were defined as volume fractions of the corresponding phase, so that material properties can be described as a function of temperature and phase fraction.

One of the important aspects considering the thermal analyses during heat treatment of steels is the heat generation due to phase transformations, which has a significant effect on the temperature profile during the heat treatment of steel. The subroutine "HETVAL" was used in this study to describe the term $\dot{Q}$ from Eq. (1). Using the incremental notation the term $\dot{Q}$ can be expressed as in Eq. (2):

$$\Delta Q_{t+\Delta t} = \frac{\Delta H_{i\to k} \Delta\xi_k \rho_k}{\Delta t} \tag{2}$$

where $\Delta Q_{t+\Delta t}$ is the incremental heat generation due to a phase transformation $i \to k$. $\Delta H_{i\to k}$ is the enthalpy difference between phase i and k, $\Delta\xi_k$ is the incremental change of the phase k. ρ_k is the density of phase k and Δt is the time increment.

2.2. Modeling the phase transformations

Phase transformations occurring during heat treatment of steels can be categorized in two major categories namely diffusionless (martensitic) and diffusion induced transformations. Phase transformations considered in this study are represented in Table 1.

In this terminology, the "phases" which are appearing during austenitization, quenching and tempering are not phases in a thermodynamic sense, but phase mixtures composed of a matrix and carbides. This terminology reflects the procedure in finite element modelling. Thus, we urge the reader to treat the term "phase" as a microstructural constituent having significantly different physical properties. These "phases" can be considered to transform. Moreover, one should also note that the term "transformation" is also used in a different meaning due to the change of physical properties. Transformations in this study generate alteration of specific volume, material properties and enthalpy, which are the decisive aspects of the phase transformation in macroscopic scale which influence the development of temperature, displacement and stresses during the heat treatment.

Phase transformations during tempering are the concern of this study. Volume changes associated with the microstructural evolution during heating to the tempering temperature can be observed by dilatometer tests [14,26]. For the steel of interest, there was no significant change observed in volume during heating up till to 450 °C for the tempering step [15,39]. Due to the higher percentage of alloying elements in steel AISI H13, martensite can maintain its tetragonality to higher temperatures of 450 °C and even 500 °C [27]. In this work, it is assumed that when heating up to tempering temperature above 450 °C, martensite and bainite transforms to

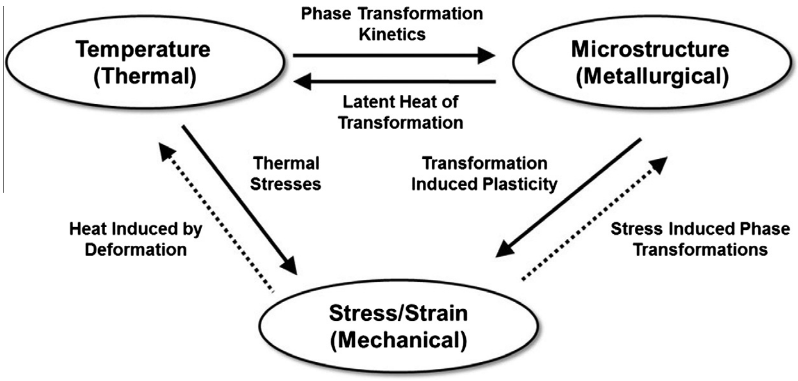

Fig. 1. Metallo-thermo-mechanical model.