Mechanics of Materials 102 (2016) 7–14

Contents lists available at ScienceDirect

Mechanics of Materials

journal homepage: www.elsevier.com/locate/mechmat

Research paper

A reduced multiscale model for heat treatments in multiphase steels

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ARTICLE INFO

Article history:
Received 15 March 2016
Revised 8 August 2016
Available online 10 August 2016

Keywords:
Multiscale analysis
Reduced model
Asymptotic expansion homogenisation
Periodic microstructure
Heat treatments

ABSTRACT

Multiphase steels offer impressive mechanical properties. However, their characterisation still represents a challenge. In a quenching processes, phenomena such as undesirable strains or residual stresses are inevitable and can be the cause for non-admissible final parts.

In this work, a reduced multiscale model is proposed, being capable of accounting phenomena such as viscous effects and phase transformations. The existence of two distinct scales is assumed, defining a micro- and a macroscale. In the smaller scale, the evolution of a steel periodic microstructure is analysed in detail and Micro-Macro (M-M) instantaneous constitutive matrices are established for macroscopic use. These matrices are established using the asymptotic expansion homogenisation methodology, allowing to predict the macrostrutural response (macroscale) based on the microstructure (microscale) information.

1. Introduction

Steels are widely used on many applications and some of them require heat treating the material in order to achive the desired strength, machinability or formability (Caseiro et al., 2011). During quenching, hardenable steels may suffer dramatic changes in their microstructure and, consequently, in their properties. Such processes may lead to the appearance of undesirable effects, such as residual stresses and distortions on the steel part (Hashmi et al., 2014). However, the quantification of the unwanted effects still represents a challenge. The non-existence of efficient non-destructive experimental procedures capable of measuring them leads to the need of numerical tools capable of quantifying these undesirable effects. During a heat treatment, inhomogeneous cooling is frequent and, when allied with phase transformations, is the source of the problems. For instance, macroscopic anisotropy in the mechanical, thermomechanical and thermal behaviours cannot be accurately modelled by classical homogeneous models, which cannot account for arbitrary distributions of constituents that may result in different types of anisotropy. In order to overcome these difficulties, the microstructure provides crucial information that should be used to model the macroscopic behaviour. This means that macroscopic anisotropy in the mechanical, thermomechanical and thermal behaviours should be modelled by appropriated averages of the microstructure domain. Additionally, the averaging process must be capable of accounting for the properties heterogeneity in the macroscopic domain as well as its arbitrary and evolutive distribution in space and time. Taking into account that thermomechanical processes such as heat treatments may increase the anisotropy of a material Harrigan and Mann (1984), its quantification is important. Some methods can be found to establish anisotropic models from a microstructure analysis. For instance, planar methods such as Saltykov or Hilliard methods Harrigan and Mann (1984) can be used, being developed for particular grain orientations. Another approach is the modification of the effective medium models to include anisotropy. For example, in 1990, Gavazzi and Lagoudas proposed the numerical solution to the analytical model of Eshelby (C.Gavazzi and Lagoudas, 1990). Later, in 2002, Wu, and Herzog proposed the use of effective properties calculated from experimental tests (Wu and Herzog, 2002). However, the previous models are developed for particular cases of anisotropy and, consequently, their applicability is limited.

Considering that microstructural evolution can be represented by a periodic spatial repetition of a Representative Unit Cell (RUC), the Asymptotic Expansion Homogenisation (AEH) is the most expedite averaging process to establish equivalent material models for macroscopic use, according to Auriault (2002). Thus, anisotropic effects are analysed microstructurally and used macrostructurally. Moreover, this methodology can account for different types of anisotropy and deal with evolutive microstructures. This mathematical homogenisation methodology of the AEH, pioneered by Bensoussan et al. (1978), emerged in 1978. Then, many authors followed this subject, as Sanchez-Palencia (1970), Guedes and Kikuchi (1990), Hollister and Kikuchi (1992), Terada and

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http://dx.doi.org/10.1016/j.mechmat.2016.08.004
0167-6636/

Kikuchi (1996), Chung et al. (2001), Yuan and Fish (2008), Pinho-da Cruz (2007), Zhang et al. (2007), Özdemir et al. (2008), Goupee and Vel (2010), and Terada et al. (2010).

As shown in previous publications Barroqueiro et al. (2016); 2015), AEH is capable of modelling a heat treatment. However, if the non-linear regime is introduced, the microscale needs to be solved in every calculation point of the macroscale in every iteration at each time increment. This approach leads to large amounts of computation, losing its practical applicability (Terada, 1996). However, AEH is capable of providing instantaneous constitutive matrices for the mechanical, thermomechanical and thermal behaviours of a material (Barroqueiro et al., 2016). Therefore, a multiscale model is presented, containing two distinct scales: a microscale and a macroscale. The macroscale consists in a phenomenological thermoelastic-viscoplastic constitutive model ruled by a set of instantaneous constitutive matrices, while the microscale, represented by a RUC, is used to provide the referred matrices needed at the macroscale.

The presented model has not been used yet to model heat treatment processes. Moreover, this non-conventional approach is able to deal with microstructural phase transformations in an expedite way. Within this work, a methodology to reduce computational costs is presented. The temperature and a material database technique are the key parameters to achieve it. While this work proposes a new approach, this topic has also been studied by other authors. Temizer and Wriggers (2007), proposed the use of the eigenvalues of the macroscopic strain tensor and their orientation as a way to construct a material map and therefore reduce computational costs. Yvonnet et al. (2013), in 2013, also proposed the use of a material database that stores the effective strain energy density functions in the macroscopic right Cauchy-Green strain tensor, combined with a simplified interpolation scheme. In this work, the presented transient multiscale model is implemented in the commercial Computer-Aided Engineering (CAE) software ABAQUS (Sorensen and and, 2010). This work also provides engineers and/or new researchers with a methodology to create their own transient multiscale model.

2. Multiscale model

This section presents the mechanical, thermomechanical and thermal models as well as the calculation process of the instantaneous constitutive matrices. These matrices provide the anisotropy models for the macroscale and their computation uses the asymptotic expansion homogenisation process and corresponds to a detailed analysis of the microscale domain (microstructure). The resultant matrices are represented with the superscript h.

2.1. Macroscopic thermal model

The two-dimensional macroscopic thermal model written in Cartesian coordinates is mathematically given by

$$\frac{\partial}{\partial x}\left(k^{\mathrm{h}}_{\mathrm{xx}}\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k^{\mathrm{h}}_{\mathrm{yy}}\frac{\partial T}{\partial y}\right)=\rho^{\mathrm{h}}c^{\mathrm{h}}\frac{\partial T}{\partial t}\,, \tag{1}$$

where ρ^{h} and c^{h} are the density and the specific heat, respectively. $k^{\mathrm{h}}_{\mathrm{xx}}$ and $k^{\mathrm{h}}_{\mathrm{yy}}$ are the effective thermal conductivity. All these properties will be defined bellow. Finally, T and t are the temperature and time, respectively.

2.2. Macroscopic thermoelastic-viscoplastic mechanical model

The macroscopic mechanical model presented in this section corresponds to an extension of the algorithm presented in Crisfield (1997) and considers phenomena such as elastic, plastic and thermal anisotropy, mixed hardening, viscous effects and anisotropic thermal expansion. Thus, in the viscoplastic regime, the constitutive equation of the stress rate is mathematically given by

$$\dot{\sigma}_{ij}=D^{\mathrm{evp}}_{ijkl}\dot{\epsilon}_{kl}\,, \tag{2}$$

where D^{evp}_{ijkl} are the thermoelastic-viscoplastic consistent moduli and

$$\dot{\epsilon}_{ij}=\dot{\epsilon}^{\mathrm{e}}_{ij}+\dot{\epsilon}^{\mathrm{th}}_{ij}+\dot{\epsilon}^{\mathrm{vp}}_{ij} \tag{3}$$

is the strain rate due to the elastic, thermal and viscoplastic components. The elastic and thermal strain rate are, respectively, defined by

$$\dot{\epsilon}^{\mathrm{e}}_{ij}=\left(D^{\mathrm{h}}\right)^{-1}_{ijkl}\dot{\sigma}_{ij}\quad\text{and} \tag{4}$$

$$\dot{\epsilon}^{\mathrm{th}}_{ij}=\left(D^{\mathrm{h}}\right)^{-1}_{ijkl}\beta^{\mathrm{h}}_{kl}\dot{T}=\alpha^{\mathrm{h}}_{ij}\dot{T}\,, \tag{5}$$

where D^{h}_{ijkl} and β^{h}_{ij} are instantaneous constitutive tensors, whose information can be retrieved by the microscale and $\dot{T}$ is temperature rate. The viscoplastic strain rate is defined by

$$\dot{\epsilon}^{\mathrm{vp}}_{ij}=\gamma\langle\Phi\rangle\frac{\partial f}{\partial\sigma_{ij}}\,, \tag{6}$$

where γ is the viscosity parameter and

$$\begin{aligned}\langle\Phi\rangle&=0\,,\quad\forall f\le 0\,,\\ \langle\Phi\rangle&=\Phi\,,\quad\forall f>0\,.\end{aligned} \tag{7}$$

Φ is the viscoplastic law and f is the yielding function, being, respectively, given by

$$\Phi=\left(\frac{\sigma_{\mathrm{e}}}{\sigma_{\mathrm{y}}}-1\right)^{N}\quad\text{and} \tag{8}$$

$$f=\sigma_{\mathrm{e}}-\sigma_{\mathrm{y}}\,, \tag{9}$$

where N is macroscopic material constant. σ_{y} is the flow stress and σ_{e} is the equivalent stress, defined by

$$\sigma_{\mathrm{e}}=\sqrt{\frac{1}{2}(\sigma_{ij}-\varpi_{ij})P_{ijkl}(\sigma_{kl}-\varpi_{kl})}\,, \tag{10}$$

where ϖ_{ij} is the backstress tensor and P_{ijkl} is a tensor of macroscopic material constants to account for anisotropy. The Hill's criterion Crisfield (1997) can be easily used to characterise the plastic anisotropy of the material. However, their coefficients must be retrieved having in account the microstructural behaviour of the material. The kinematic and isotropic hardening laws are

$$\dot{\varpi}_{ij}=\frac{K\Phi}{\sigma_{\mathrm{e}}}(\sigma_{ij}-\varpi_{ij})\quad\text{and} \tag{11}$$

$$\sigma_{\mathrm{y}}=\sigma^{\mathrm{h}}_{0}+H\Phi\,, \tag{12}$$

respectively, where H and K are the macroscopic hardening rates of the material and σ^{h}_{0} is the macroscopic flow stress, corresponding to the volumetric average of yield stresses of the microscale constituents.

2.3. Micro-Macro instantaneous constitutive matrices

The instantaneous constitutive matrices are evaluated using the asymptotic expansion homogenisation methodology over the microscale domain Y. The referred domain represented by a periodic RUC is temperature-dependent and, consequently, time-dependent. This means that different points of the macroscale might use different RUCs, as illustrated by Fig. 1. Therefore, each calculation