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Multiscale analysis of heat treatments in steels: Theory and practice

B. Barroqueiro*, J. Dias-de-Oliveira, J. Pinho-da-Cruz, A. Andrade-Campos

Department of Mechanical Engineering, Centre for Mechanical Technology & Automation, GRIDS Research Group, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal

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ABSTRACT

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

In this work, a numerical multiscale transient model, that uses the Asymptotic Expansion Homogenisation (AEH) methodology combined with Finite Element Method (FEM), is proposed for the analysis of heat treatments in steels. The implementation of the AEH method is carried out using the commercial program Abaqus, considering an uncoupled and transient problem with implicit time integration. Within the homogenisation method, 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 an equivalent homogeneous material model is established for macroscopic use. Moreover, it is presented in this work that AEH is a rigorous and effective homogenisation method that allows the modelling of the thermomechanical and transient thermal behaviour in periodic materials, particularly in heat treatments.

1. Introduction

Steels are widely used on many applications and some of them require heat treating the material in order to achieve the desired strength, machinability or formability [1]. During quenching, hardenable steels may suffer dramatic changes in their microstructure and, consequently, on their properties. Such processes may lead to the appearance of undesirable effects such as residual stresses and distortions on the steel part [2]. The residual stresses have their origin on plasticity phenomena and phase transformations. Moreover, inhomogeneous cooling processes tend to intensify the unwanted effects. Nowadays, there is little doubt that steel phase transformations play a major role in the development of residual stresses and should be taken into account [3]. Therefore, this work presents a transient multiscale model capable of reproducing the thermomechanical behaviour in the referred transformations using the Asymptotic Expansion Homogenisation (AEH) methodology and Finite Element Method (FEM).

Homogenisation is rapidly maturing due to the increasing power of computation. However, this subject dates back to many years ago, starting with homogenisation methods such as effective medium models of Eshelhy [4], Mori and Tanaka [5], self-consistent approaches of Hill [6] and many others [7]. Later, a new mathematical homogenisation methodology emerged as the Asymptotic Expansion Homogenisation pioneered by Bensoussan et al. [8].

Many authors followed this subject, as Sanchez-Palencia [9], Guedes and Kikuchi [10], Hollister and Kikuchi [11], Terada and Kikuchi [12], Chung et al. [13], Yuan and Fish [14], Pinho-da-Cruz et al. [15], Zhang et al. [16], Özdemir et al. [17], Goupee and Vel [18], and Terada et al. [19]. For instance, Zhang et al. [16] used a thermomechanical multiscale model in order to model the thermodynamic wave propagation phenomena. Özdemir et al. [17] also used a thermomechnical multiscale with particular emphasis in modelling thermal shocks and consequent thermomechanical damage and debonding. Later, Terada et al. [19] also used a thermomechanical multiscale model with microscale heat transfer in order to analyse porous solids.

The base formulation of the presented multiscale model has been used by other authors in order to model many phenomena, as previously enumerated. However, the modelling of steel heat treatments with phase transformations provides a new application.

* Corresponding author. Tel.: +351 234 370830; fax: +351 234 370933.
E-mail addresses: bjfb@ua.pt (B. Barroqueiro), jalex@ua.pt (J. Dias-de-Oliveira), jpc@ua.pt (J. Pinho-da-Cruz), gilac@ua.pt (A. Andrade-Campos).

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The presented transient multiscale model is implemented in the commercial Computer-Aided Engineering (CAE) software ABAQUS [20]. This provides engineers and/or new researchers with a methodology to create their own transient multiscale model. This is taken further with a code subroutine that is provided in Appendix A, in order to facilitate and encourage new developments.

The AEH methodology considers the existence of two distinct scales: a micro- and a macroscale. During the process, the macroscale is explicitly analysed using the information gathered on a detailed analysis of the microscale. Being a multiscale procedure, the inverse approach is also done. The detailing of the material behaviour in the microscale with the results from the macroscale is called localisation. This homogenisation methodology allows the analysis of a great number of different microstructures, given the requirement of a periodic Representative Unit Cell (RUC) [21]. The main advantages of this methodology are: (i) allowing the modelling of the mechanical, thermomechanical and transient thermal behaviours of periodic materials with a rigorous and effective homogenisation methodology, (ii) reducing the number of degrees of freedom linked to modelling of the material behaviour, (iii) allowing the proper characterisation of periodic heterogeneous microstructures [15] and (iv) analysing the material anisotropy microstructurally for macroscopic use. However, this methodology has drawbacks. If non-linear phenomena (*i.e.* phase transformations) are introduced, several of microscales are needed, since each material point of the macroscale might evolve in a particular way. Therefore, techniques to reduce the computational costs are needed. Within this work, a methodology to reduce computational costs is presented and the temperature is a key parameter to achieve it. While this work proposes a new approach, this topic has also been studied by other authors. Temizer and Wriggers [22], 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. [23], 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.

This document starts with the introduction of the transient multiscale model formulation, its assumptions and differential formulation, followed by the analysis and discussion of the finite element formulation of the variational problems and their implementation. Then, a validation test is presented, where AEH methodology is compared to the general FEM methodology. In the end, a multiscale application of AEH in heat treatments and its results, such as the characteristic displacement fields, the homogenised properties, the stress and temperature evolution, and the process of localisation for both mechanical and thermal fields, are presented. Finally, some final remarks are provided.

2. Asymptotic Expansion Homogenisation

2.1. Initial considerations

The Asymptotic Expansion Homogenisation is an homogenisation methodology capable of modelling the behaviour of periodic materials in an uncoupled and quasi-static process. The macroscopic behaviour of a heterogeneous material is derived from the heterogeneity scale that describes the physical process over a Representative Unit-Cell (RUC) [21], *i.e.*, the spatial repetition of the RUC form the heterogeneous material. However, the referred element has to be large enough to represent the material and small enough when compared to the macroscopic volume. The fundamental condition can be expressed as

$$\epsilon = \frac{l}{L} \ll 1, \tag{1}$$

where l and L are the characteristic lengths of the RUC and macroscopic body, respectively. In the presence of a periodic heterogeneous medium, the AEH is the most effective methodology [24]. At this point, it is common to assume two distinct scales: $\mathbf{x}$ and $\mathbf{y}$ for the behaviour of the materials in the macroscale and in the microscale, respectively [7]. Thus, the variables related to the referred fields become functionally dependent on both $\mathbf{x}$ and $\mathbf{y}$ scales, where

$$\mathbf{y} = \mathbf{x}/\epsilon. \tag{2}$$

The referred functional dependence is usually called Y-periodicity. Thereby, the Y-periodicity of the microstructural heterogeneities reflects itself on the fact that the thermal expansion tensor $\boldsymbol{\alpha}$, the elasticity tensor $\mathbf{D}$ and the thermal conductivity tensor $\mathbf{k}$ are Y-periodic in $\mathbf{y}$. In contrast, the material homogeneity at the macroscale level results from the fact that the tensors do not depend on the macroscale $\mathbf{x}$, resulting in

$$\alpha_{ij} = \alpha_{ij}(\mathbf{y}), \tag{3}$$

$$D_{ijkl} = D_{ijkl}(\mathbf{y}) \quad \text{and} \tag{4}$$

$$k_{ij} = k_{ij}(\mathbf{y}). \tag{5}$$

On the macroscale $\mathbf{x}$, the microscale constituents appear over periods ϵ^{-1} times smaller than the characteristic dimension of Y. Replacing Eq. (2) in Eqs. (3)–(5) results in

$$\alpha_{ij}^{\epsilon} = \alpha_{ij}(\mathbf{x}/\epsilon), \tag{6}$$

$$D_{ijkl}^{\epsilon} = D_{ijkl}(\mathbf{x}/\epsilon) \quad \text{and} \tag{7}$$

$$k_{ij}^{\epsilon} = k_{ij}(\mathbf{x}/\epsilon), \tag{8}$$

respectively, where the superscript ϵ states that $\boldsymbol{\alpha}$, $\mathbf{D}$ and $\mathbf{k}$ are ϵY-periodic in the macroscale $\mathbf{x}$.

The formulation presented in the following sections is based on the formulations presented in [13,15,25,26].

2.2. Homogenisation of thermoelastic problem

Assuming infinitesimal strains and a quasi-static process, the linear thermoelastic problem is given by the following equations:

$$\frac{\partial \sigma_{ij}^{\epsilon}}{\partial x_j^{\epsilon}} + f_i = 0 \quad \text{in } \Omega, \tag{9}$$

$$\varepsilon_{ij}^{\epsilon} = \frac{1}{2}\left(\frac{\partial u_i^{\epsilon}}{\partial x_j^{\epsilon}} + \frac{\partial u_j^{\epsilon}}{\partial x_i^{\epsilon}}\right) \quad \text{in } \Omega \text{ and} \tag{10}$$

$$\sigma_{ij}^{\epsilon} = D_{ijkl}^{\epsilon}\varepsilon_{kl}^{\epsilon} - \beta_{ij}^{\epsilon}\Delta T^{\epsilon}, \tag{11}$$

where

$$\Delta T^{\epsilon} = T^{\epsilon} - T_0 \quad \text{and} \tag{12}$$

$$\beta_{ij}^{\epsilon} = D_{ijkl}^{\epsilon}\alpha_{kl}^{\epsilon} = \beta_{ij}(\mathbf{x}/\epsilon). \tag{13}$$

σ_{ij}^{ϵ} and $\varepsilon_{ij}^{\epsilon}$ are the components of the Cauchy stress and the strain tensors, respectively. f_i, u_i and T_0 are the loads per unit of volume, displacements and the reference temperature, respectively. The boundary of Ω is defined by the surfaces Γ_D and Γ_N . These are related to the Dirichlet and Neumann boundary conditions