International Journal of Engineering Science 127 (2018) 92–113

Contents lists available at ScienceDirect

International Journal of Engineering Science

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

FFT-based modelling of transformation plasticity in polycrystalline materials during diffusive phase transformation

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ARTICLE INFO

Article history:
Received 12 January 2017
Accepted 11 February 2018
Available online 20 March 2018

Keywords:
Transformation plasticity
Steel
FFT
Crystal plasticity

ABSTRACT

During heat treatment processes of steel products, transformation plasticity is known to play an important role as it affects the final product quality such as shape and residual stresses. To investigate this well-known phenomenon, a model coupling crystal plasticity with diffusive phase transformation is developed by using a fast Fourier transform (FFT) numerical scheme. Diffusional transformation including a plastically accommodated volume change is considered (i.e. the Greenwood–Johnson mechanism). The model is then used to determine the pre-hardening effect on transformation plasticity. It is revealed that pre-hardening results in an anisotropic transformation strain; pre-tension decreases transformation strain and pre-compression increases transformation expansion along the pre-hardened direction. The model is also used to assess the existing analytical model developed by Leblond and Taleb. In this attempt, some features that contribute to the transformation plasticity are discussed. Among those, it is found that plastic deformation in daughter phase is non-negligibly small especially in the end of phase transformation. These analytical solutions predict linear relation between applied stress and transformation plastic strain. This reasoning attributes the linear relation to the solution of equivalent plastic strain increase with transformation by only the transformation expansion effect neglecting the applied stress effect

1. Introduction

During the thermomechanical treatments involved in steel processing, transformation plasticity or transformation induced plasticity (TRIP) occurs as a result of the variation of the volumic fraction of the phases during the solid state transformation. Two main mechanisms are classically invoked: (i) a *displacive* mechanism (i.e. Magee effect (Magee, 1966)) with a *shape change* during transformation and (ii) a *diffusive* mechanism (i.e. Greenwood–Johnson effect (Greenwood & Johnson, 1965)), implying nucleation and growth steps, with a *volume change* plastically accommodated (Fischer, Sun, & Tanaka, 1996). They both have been the subject of a number of experimental studies (see, among others Boudiaf, Taleb, & Belouchrani, 2011; Desalos, 1981; Gautier, Simon, & Beck, 1987; Holzweissig, Canadinc, & Maier, 2012; Lambers, Tschumak, Maier, & Canadinc, 2010; Petit-Grostabussiat, Taleb, & Jullien, 2004; Taleb, Cavallo, & Waeckel, 2001).

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https://doi.org/10.1016/j.ijengsci.2018.02.008

The phenomenon is known to play a central role during phase transformation in defining the final shape and residual stress state of heat treated materials. Phenomenological models have been developed and been used in the framework of finite element thermo-mechanical simulations (Inoue, Wang, & Miyao, 1987-5; Ju, Zhang, & Zhang, 2006; Montalvo-Urquizo, Liu, & Schmidt, 2013).

The micromechanical modelling of transformation plasticity dates back to the pioneering theoretical work of Leblond, Mottet, and Devaux (1986) based on a rigorous homogenisation procedure. Few years later, an approximate analytical model has been derived from (Leblond, 1989; Leblond, Devaux, & Devaux, 1989) to describe transformation plasticity due to the Greenwood–Johnson mechanism. Since then, developments have been suggested based on this approach (Taleb & Sidoroff, 2003). Besides, it is worth mentioning that a variety of mean-field models have been developed; see, for instance, Cherkaoui, Berveiller, and Lemoine (2000), Diani, Sabar, and Berveiller (1995) and Fischlschweiger, Cailletaud, and Antretter (2012). Apart from these works, numerical micromechanical modelling has also been performed, making use of the finite-element method (FEM) to study diffusional transformations. With increasing complexity, numerical investigations have first considered the case of a two-phase material with J_2 plasticity, and various nucleation rules (Barbe, Quey, & Taleb, 2007; Barbe, Quey, Taleb, & Souza, 2008; Ganghoffer, Denis, Gautier, & Simon, 1993; Leblond et al., 1986; Leblond et al., 1989), and more recently, the case of polycrystalline materials with crystalline plasticity at the slip system level, together with a microstructure described by a Poisson-Voronoi tessellation (Barbe & Quey, 2011).

In the context of *classical plasticity* (i.e. without solid phase transformation), an efficient numerical scheme based on fast Fourier transform (FFT) (Moulinec & Suquet, 1998) has been successfully applied to a variety of problems and constitutive relations (Brenner, Lebensohn, & Castelnau, 2009; Lebensohn, Kanjarla, & Eisenlohr, 2012; Lebensohn, Brenner, Castelnau, & Rollett, 2008; Lee, Lebensohn, & Rollett, 2011; Suquet et al., 2012). This alternative approach to FEM allows to consider large polycrystalline aggregates with reasonable CPU time and memory allocation. Its accuracy has been discussed by confronting with FEM simulation results (Eisenlohr, Diehl, Lebensohn, & Roters, 2013). Besides, meshing of the microstructure is not necessary as the computation is directly made on the digital image of the material (regular grid of pixels in 2D or voxels in 3D). These features are especially convenient to consider experimental microstructural data obtained by fine-scale EBSD or X-ray diffraction contrast tomography (Belkhabbaz, Brenner, Rupin, Bacroix, & Fonseca, 2011; Grennerat et al., 2012; Ludwig, Schmidt, Lauridsene, & Poulsen, 2008). By contrast to FEM, the FFT method is limited to a periodic homogenisation scheme which makes it less general.

In the present work, we first investigate the application of the FFT method in the context of plasticity induced by diffusional transformation. Following previous investigation, an enhanced numerical scheme is employed incorporating the pre-hardening effect, which induces the back stress and thus the anisotropic effect on transformation plasticity. Then, use is made of FFT reference results on representative polycrystalline aggregates for a critical analysis of two existing analytical micromechanical models (Leblond et al., 1989; Taleb & Sidoroff, 2003). These analytical models are compared for varying material data (transformation expansion coefficient).

2. Formulation of FFT-based numerical scheme

The FFT numerical scheme proposed by Moulinec and Suquet (1998) relies on the Green functions method to solve a periodic boundary value problem for heterogeneous media. For completeness, its formulation is first recalled. It offers a straightforward framework to consider stress-free strains related to the solid-state transformation process. Then, the constitutive local equations for crystalline plasticity and transformation kinetic are detailed.

2.1. Lippmann-Schwinger equation for periodic media

2.1.1. Formulation

In the case of a periodic boundary problem, the local displacement can be divided into fluctuation and average terms such that:

$$\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{u}'(\boldsymbol{x}) + \bar{\varepsilon}\boldsymbol{x} \tag{1}$$

where, $u'(x)$ is a periodic displacement. The strain field reads:

$$\boldsymbol{\varepsilon}(\boldsymbol{u}(\boldsymbol{x})) = \boldsymbol{\varepsilon}(\boldsymbol{u}'(\boldsymbol{x})) + \bar{\varepsilon} \tag{2}$$

with $\langle \boldsymbol{\varepsilon}(\boldsymbol{u}'(\boldsymbol{x}))\rangle = 0$.

For a heterogeneous elasto-plastic material, the rate-form of constitutive relation reads:

$$\dot{\boldsymbol{\sigma}}(\boldsymbol{x}) = \boldsymbol{C}(\boldsymbol{x}) : \dot{\boldsymbol{\varepsilon}}^e(\boldsymbol{x}) = \boldsymbol{C}(\boldsymbol{x}) : \left(\dot{\boldsymbol{\varepsilon}}(\boldsymbol{x}) - \dot{\boldsymbol{\varepsilon}}^p(\boldsymbol{x}) - \dot{\boldsymbol{\varepsilon}}^m(\boldsymbol{x})\right) \tag{3}$$

where $\boldsymbol{C}(x)$ is the elastic tensor at local position x and ε^e, ε, ε^p and ε^m are elastic, total, plastic and transformation strain tensor respectively. Equivalently, the constitutive law can be rewitten:

$$\dot{\boldsymbol{\sigma}}(x) = \boldsymbol{C}(\boldsymbol{x}) : \dot{\boldsymbol{\varepsilon}}(\boldsymbol{x}) + \dot{\boldsymbol{\tau}}(\boldsymbol{x}) \tag{4}$$