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A macroscale phase-field model for shape memory alloys with non-isothermal effects: Influence of strain rate and environmental conditions on the mechanical response

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Abstract

A Ginzburg–Landau model for the macroscopic behaviour of a shape memory alloy is proposed. The model is essentially one-dimensional, in that we consider the effect of the martensitic phase transition in terms of a uniaxial deformation along a fixed direction and we use a scalar order parameter whose equilibrium values describe the austenitic phase and the two martensitic variants. The model relies on a Ginzburg–Landau free energy defined as a function of macroscopically measurable quantities, and accounts for thermal effects; couplings between the various relevant physical aspects are established based on thermodynamic principles. The theoretical model has been implemented within a finite-element framework and a number of numerical tests are presented which investigate the mechanical behaviour of the model under different conditions; the results obtained are analyzed in relation to experimental evidence available in the literature. In particular, the influence of the strain rate and of the ambient conditions on the response of the model is highlighted.

Keywords: Phase field model; Shape memory alloys; Strain-rate sensitivity; Thermo-mechanical coupling

1. Introduction

Shape memory alloys (SMAs) have many applications and are attracting much interest due to their unique properties of shape memory and pseudoelasticity, which stem from both temperature-induced and stress-induced martensitic phase transition. The mechanical behaviour of such materials is rather complex and arises from a strong interaction between thermal and mechanical phenomena. In fact, when these materials undergo the martensitic phase transition, the changes in temperature due to localised self-heating/self-cooling has been experimentally found to be anything but negligible [1–4]. Hence, the effects of heat transfer and of heat dissipation towards the ambient are of primary relevance in the study of these materials [2,5] and play a role in the rate-dependent behaviour of SMAs [3,6].

In modelling the mechanical behaviour of a SMA it is therefore important to account for mechanical and thermal aspects at the same time and to evaluate the evolution with time of all phenomena.

Many constitutive models for SMAs, derived from a variety of approaches, exist in the literature [7]. Some authors propose models developed within plasticity frameworks, which make use of one or even more internal variables to describe the pseudo-elastic behaviour [8–10]. Another group of constitutive models has been developed within a thermomechanic context; in his work, Tanaka [11] proposed a macroscale model comprising an internal variable to quantify the extent of the phase transition, a

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dissipation potential and an assumed transformation kinetic. Similarly, other models based on the same thermodynamic background but featuring different kinetic laws have been formulated [12,13], and a complete heat equation which accounts for the contribution of latent heat and of the dissipation connected with the phase transition was added to the framework [14,15]. Among others, Chang et al. [16] proposed a model comprising a strain-gradient elastic free energy and a chemical (transitional) free energy; Abeyaratne et al. [17] developed a model including a non-convex Helmholtz free energy function of the strain in order to describe the regions of stability of the different phases. Furthermore, some micromechanical models have been proposed [18–21]. Patoor et al. [18] and Sun and Hwang [19] developed models based on thermodynamic considerations for polycrystalline SMAs in which the free energy is a function of the deformation and of the volumetric fraction of the phases involved, while Müller and Seelecke [21] developed a microscale model based on statistical physics comprising a non-convex bulk free energy function of the lattice shear deformation.

Another approach to the description of the behaviour of SMAs consists in applying the Ginzburg–Landau theory for phase transitions. At a microscopic scale, Falk [22] developed a Landau theory based on a shear strain order parameter. Levitas and Preston [23] proposed a single-grain model based on the decomposition of the strain in an elastic and a transformational part, the latter being described by a pure order parameter which can assume different values to identify the different phases. In a similar fashion, Wang and Khachaturyan [24] proposed a model in which the strain field depends on several order parameters, whose evolution is described by several time-dependent Ginzburg–Landau (TDGL) equations. Nevertheless, attempts to handle the problem at a larger scale of observation have been made as well. Among others, Ahluwalia et al. [25] and Chen and Yang [26] proposed mesoscale models for the description of polycrystalline materials in which the order parameters account for the different orientations of each single grain; in the same spirit, Brocca et al. [27] proposed a microplane model attempting to bridge the gap between micromechanics-based and macroscale models. At the macroscopic scale, He and Sun [28,29] developed a model based on a non-convex bulk free energy function of the strain and a strain-gradient part in order to account for interfaces between the phases. In addition, Berti et al. [30] proposed a Ginzburg–Landau model which can be applied at the macroscale and encompasses mechanical as well as thermal effects by introducing the balance of linear momentum equation and the heat equation in a thermodynamically consistent framework; the order parameter is related to the extent of the phase transition between austenite and the martensite variants and its evolution is regulated by a TDGL equation. Owing to the presence of the heat equation, it is possible to describe the thermomechanical interactions which strongly influence the constitutive behaviour of a SMA and to account for non-isothermal conditions. The model is presented both in a three-dimensional and a monodimensional setting; the reduction to this latter case is still meaningful because in most engineering applications SMA wires are employed.

In this paper, we present a numerical study on the thermomechanical behaviour of a SMA, with a particular focus on the rate-dependent response and on the influence of thermal conduction and heat transfer on the mechanical behaviour. Starting from the models proposed in Berti et al. [30] and Daghia et al. [31], we formulate a new free energy functional and give a proper expression for the relaxation parameter regulating the TDGL equation; this gives the model the properties required to reproduce the symmetric behaviour between the austenite-to-martensite and the martensite-to-austenite phase transitions observed experimentally. The ability of the model to quantitatively reproduce a variety of experimental evidences of a typical polycrystalline NiTi alloy is then demonstrated.

The paper is organised as follows. In Section 2, the theoretical model is described, starting from a suitable Ginzburg–Landau free energy whose properties are outlined in Section 2.1. Constitutive relations are given in Section 2.2, while the thermodynamic consistency of the model is shown in Section 2.3 and the complete differential system with appropriate boundary and initial conditions is provided in Section 2.4. In Section 3 the Galerkin formulation of the differential problem, suitable for the finite-element implementation, is sketched. Section 4 is the main part of the paper, where the numerical results of a number of simulated tensile tests on a bar specimen under different conditions are reported. After describing, in Section 4.1, the effectiveness of the model in recovering the main experimental evidences in terms of stress–strain response, phase morphology and temperature evolution, in Section 4.2 tensile tests performed at different values of the initial temperature are illustrated, while in Section 4.3 the stress–strain response under partial-loading conditions is depicted. The rate-dependent behaviour of the model is investigated in Section 4.4, with a particular focus on the effects of the strain rate on the domain nucleation, the hysteresis cycle and the energy dissipation. The influence of heat transfer phenomena on the mechanical response of the specimen is examined in Section 4.5. The last two aspects are considered jointly in Section 4.6. The paper ends by drawing some conclusions in Section 5.

2. Model

The thermomechanical properties of SMAs stem from the nature of the martensitic phase transition; here we will account for it by means of a Ginzburg–Landau approach [22,23]. To this end we have to define a phase field, or order parameter, φ; unlike the approach followed, among others, by Falk [22], the order parameter is not identified with the uniaxial strain ε_{11}, but rather the phase field φ is used here as a macroscopic indicator of the phase (i.e. of the microscopic structure, martensite or austenite) of the material