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Phase field study of the microstructure evolution and thermomechanical properties of polycrystalline shape memory alloys: Grain size effect and rate effect

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ABSTRACT

Shape memory alloys (SMAs) are a class of metallic smart materials which possess pseudoelasticity (PE) and shape memory effect (SME), depending on the ambient temperature. The unique thermomechanical properties of SMAs originate from the temperature-induced as well as stress-induced martensitic transformations (MTs). Former research work has shown that the thermomechanical properties of polycrystalline SMAs are grain size and rate dependent. In order to explore the physical mechanisms behind this phenomenon, a phase field (PF) model is developed in this paper to study the microstructure evolution and the thermomechanical responses of polycrystalline SMAs under dynamic loadings. The inertial effect, the latent heat release and conduction during the phase transformation are simultaneously considered. The grain boundary energy change during the phase transformation is also accounted for in the PF model. Numerical simulations are then conducted to study the temperature-induced MT as well as the stress-induced martensite reorientation of nanocrystalline SMAs with different grain sizes. The influences of the grain size, the latent heat effect and the loading rate on the microstructure evolution process and the stress–strain curves are systematically discussed.

1. Introduction

Shape memory alloys (SMAs) are a class of metallic materials that exhibit the unique characteristic of shape recovery upon appropriate thermal procedures. The excellent properties of these materials originate from a first order solid-to-solid diffusionless and reversible phase change known as martensitic transformation (MT). By applying proper thermomechanical loading, the crystal structure of these materials transforms from the high-temperature austenitic phase to the low-temperature martensitic phase with rearrangement of the atoms. Shape memory alloys can exhibit different properties in various ambient temperature ranges. For example, above the austenitic-finish temperature (A_f), the stress-induced forward MT occurs upon loading and inverse transformation occurs upon unloading. The deformation recovers completely during this process, which is referred to as pseudoelasticity (PE). Below the martensitic-finish temperature (M_f), a residual strain generates during the loading–unloading process and the material will revert to its original shape when heated, which is named shape memory effect (SME). The unique thermomechanical properties have made these materials popular in a variety of engineering applications ranging from implantable medical devices to actuators [1].

Intensive research work has been conducted in the past few decades to characterize the complex mechanical behavior of SMAs. Particularly, many efforts were dedicated to developing models that would help understand the physical mechanisms underlying the stress- and temperature-induced transformations, martensite reorientation or cyclic effects. These models can be categorized as either micro, micro–macro or macro [2]. To name a few, Sun and Hwang [3,4] developed constitutive models for polycrystalline SMAs based on the micromechanics theories. Gall et al. [5] studied the effect of stress states on the stress-induced MT in CuZnAl. Auricchio et al. [6], Auricchio and Petrini [7] and Lexcellent et al. [8] developed phenomenological constitutive models for SMAs. Lagoudas [9] and Paiva and Savi [10] presented general overviews of the phenomenological constitutive models of SMAs. Qidwai and Lagoudas [11], Panico and Brinson [12], Bhattacharya and Sadjadpour [13], and Kelley et al. [14] developed constitutive models for SMAs based on microscale deformation mechanisms. Zaki and

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Moumni [15] and Ziólkowski [16] proposed three-dimensional constitutive models for the thermomechanical behavior of SMAs. Alessi and Pham [17] developed a variational framework for the three-dimensional macroscopic modelling of superelastic shape memory alloys in an isothermal setting. Sergio et al. [18] incorporated plasticity in the constitutive description of the thermomechanical behavior of SMAs. For more thorough reviews on this topic, see Khandelwal and Buravalla [19], Lagoudas et al. [20], and Cisse et al. [21]. Besides constitutive modelling, microscopic simulations are found to be very helpful to reveal and characterize the deformation mechanisms of SMAs. For instance, Zhong et al. [22] studied PE and SME of SMAs with molecular dynamics (MD) simulations. Mirzaeifar et al. [23] performed MD simulations to study the structural transformations of the austenitic B2 to the martensitic B19′ phase in NiTi nanowires.

In recent years, the phase field (PF) method has been proved to be a powerful modelling approach to track microstructural evolution processes in materials at the mesoscale [24]. The PF method has been widely applied to study solid state phase transformations (PTs) [25–28], domain switching in ferroelastic and ferroelectric materials [29–32] and crack propagation problems [25,33–35], etc.. The application of the PF method to study the deformation mechanisms and mechanical properties of SMAs has also become very popular in these years. For instance, Wang and Khachaturyan [36] adopted the phase field microelasticity theory to simulate a generic cubic to tetragonal martensitic transformation in a prototype crystal. Artemev et al. [37] applied the very similar theory to study the proper multivariant martensitic transformations in Fe–31%Ni alloy. Bouville and Ahluwalia [38] studied the microstructure and mechanical properties of constrained single crystalline FePd nanograins and nanowires with the PF method. It was shown that the geometric constraints and boundary conditions could have significant impact on the martensite formation. She et al. [38] studied the cubic to tetragonal MT with the PF method. The influence of different initial conditions and microscopic defects was discussed in this model. Zhong and Zhu [39] developed a 3D PF model based on the Landau-type polynomial energy function to study the B2–B19′ phase transformation in nickel–titanium (NiTi) SMAs. Recently, Ahluwalia et al. [40] studied the grain size dependence of MTs and stress–strain response of nanocrystalline SMAs within the framework of the Ginzburg-Landau (GL) theory. Javanbakht and Barati [41] proposed a 2D PF model and discussed the effect of surface tension on phase transformations (PTs) in NiAl SMAs. They concluded that the surface tension could suppress the nucleation of PT.

However, all the PF models mentioned above adopted the isothermal hypothesis. Actually, a significant amount of latent heat will be released during the MT process, which will distinctly change the temperature of the material. As the mechanical properties and the hysteretic behaviors of SMAs are sensitive to temperature, it is thus necessary to consider the latent heat release and conduction in the PT process. Significant progresses have been made toward this end in recent years. To name a few, Grandi et al. [42] proposed a one dimensional PF model to investigate the influence of strain rate and environmental conditions on the mechanical response of SMA nanowires, in which the thermal effects were considered. Dhote et al. [43–47] formulated the governing equations of the temperature field and developed 2D as well as 3D coupled PF models to investigate the impact of latent heat and loading rate on the microstructural evolution and thermomechanical properties of SMAs. The strain-based order parameters are adopted in these models, which leads to the fourth-order differential equations in space. More recently, Cui et al. [48] developed a 3D non-isothermal PF model by using independent order parameters. The non-isothermal PF model was applied to investigate the latent heat and elastocaloric effects in Mn–Cu alloys. However, it is noted that all of these studies are for single crystalline SMAs.

The experimental work by Ahadi and Sun [49,50] has shown that the thermomechanical properties of SMAs as well as their fracture toughness are grain size and rate dependent. The grain size dependence of the MT and stress–strain response of nanocrystalline SMAs has been investigated by Ahluwalia et al. [40] within the framework of the Ginzburg-Landau (GL) theory. However, it is noted that the latent heat and loading rate effect were not considered in that study. In this paper, we extend the PF model presented by Dhote et al. [45–47] to the polycrystalline case. The late heat release and conduction as well as the inertial effect are accounted for in the PF model. What's more, an additional grain boundary energy term is included in the PF model to characterize the grain boundary energy change during the phase transformation process. The new PF model is then adopted to study the grain size effect and rate-dependent thermomechanical properties of SMA nanowires. The temperature-induced MT as well as the stress-induced martensite reorientation is simulated. The influences of the grain size, the latent heat effect and the loading rate on the MT and the associated stress–strain curves are systematically discussed.

The paper is organized as follows: In Section 2, the thermomechanical coupling PF model for the 2D square-to-rectangular MT is extended to the polycrystalline case by considering the grain orientation and grain boundary energy change during the PT. In Section 3, the temperature-induced phase transformation and the stress induced martensite reorientation are simulated for nanocrystalline nanowires with different grain sizes. The influence of the grain size, the latent heat effect and loading rate on the domain pattern evolution and the stress–strain curves are discussed. Finally, the conclusions are drawn in Section 4.

2. The phase field model

The unique thermomechanical properties of SMAs originate from the martensitic phase transformation and its associated martensite reorientation. The high-symmetry austenitic phase, the co-existed austenitic and martensitic phases and the low-symmetry martensitic phase are stable at high temperature, intermediate temperature and low temperature, respectively. The evolution of the phases can be characterized with the Ginzburg-Landau (GL) theory. In this paper, the representative cubic-to-tetragonal phase transformations of FePd SMA are considered. The phase field model developed by Dhote et al. [43] is briefly introduced here. After that, the phase field model is extended to the polycrystalline case.

In PF models, the order parameters are used to define the different phases in a domain. In the phase field model developed by Dhote et al. [43], the deviatoric strain e_2 directly contributed from the PT is adopted to indicate different phases: $e_2 = 0$ presents the austenite phase, while $e_2 > 0$ and $e_2 < 0$ respectively, presents

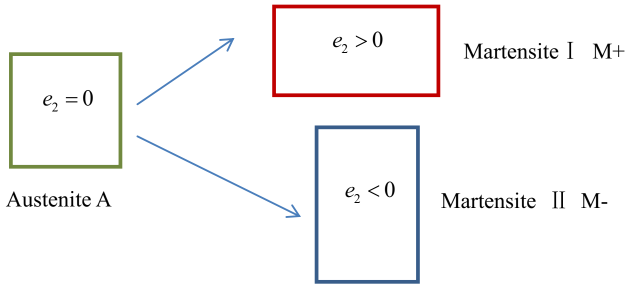

Fig. 1. The square-to-rectangular phase transformation.