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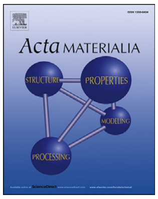

Full length article

Mesoscale simulation of elastocaloric cooling in SMA films

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ABSTRACT

A model for the evolution of the mechanical and thermal properties of shape memory alloy (SMA) films during elastocaloric cycling is developed and compared with experiments. The focus is on Ti-Ni-Cu-Co films of 20 μm thickness showing ultra-low fatigue properties. The films undergo a highly localized pseudoelastic transformation under tensile load cycling featuring strain and temperature band patterns that depend on the loading conditions. The corresponding temperature change is of special interest for film-based elastocaloric cooling applications. Starting from a thermodynamics-based Gibbs free energy model comprising mechanical and chemical contributions, we include a martensite-austenite interface free energy term, for which formulations from a phase-field model are adapted. A 3D continuum mechanics description is modified to treat plane stress conditions appropriate for polycrystalline thin films. The nucleation mechanism of strain bands under dynamic loading is described by introducing a spatial random distribution of the transformation stress barriers reflecting the degree of material inhomogeneity. Heat transfer due to conduction and convection is taken into account. The simulations predict the correlated mechanical and thermal local response of the films including band formation and evolution, tilt angle as well as strain-rate dependence. Macroscopic stress-strain characteristics and thermal evolution curves well represent the experimental results.

1. Introduction

The need for energy efficient and environmentally friendly cooling technologies has led to an increased interest in solid-state cooling based on caloric effects [1–3]. Amongst these, the elastocaloric effect is particularly promising, providing large temperature changes without the need for strong magnetic or electric fields [4,5]. Elastocaloric cooling exploits the exchange of latent heat during the diffusionless first order phase transformation between austenite (A) and martensite (M) phase in shape memory alloys (SMA) subjected to external stress [6]. The corresponding stress-strain behavior is usually referred to as pseudoelasticity or superelasticity. TiNi-based alloys offer recoverable strains of up to 10%, latent heats of up to 30 J/g and temperature change of 25–58 K under adiabatic conditions [7,8]. Recently, a number of demonstrators including heat recovery have been developed showing large cooling power and interesting values of COP exceeding 3 on the device level [9–12].

Due to favorable scaling behavior, elastocaloric cooling is well applicable for small scale applications, for example in microelectronics, bio-medical and lab-on-chip systems [13,14]. The high-surface-to-volume ratio inherent to thin films enables fast heat transfer and high cycling rates, especially for the case of narrow hysteresis [9]. However, in microscale applications the localized nature of the transformation is an important issue, as it affects the dynamics of heat release and absorption. For polycrystalline TiNi, for instance, the stress-induced pseudoelastic transformation often evolves via local strain bands being in martensitic phase, which nucleate and propagate after an initial elastic deformation. These deformation bands, called Lüders-like strain bands (LSB), are mostly observed in thin samples. Their origin was explained as morphological instability driven by local geometric defects of the material, similar to a necking instability [15]. A strong dependence of the band number on the loading rate has been found, related to the change of temperature close to the transformation front [15,16].

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For the applications in elastocaloric cooling, important challenges are the understanding and control of these local strain and temperature effects as well as the heat transfer dynamics.

The modeling of the strain band mechanism involves a tight coupling of mechanics, phase kinetics and thermal evolution as well as a pronounced hysteresis in the stress-strain behavior. As the strain rate $\dot{\varepsilon}$ and heat transfer to the environment influence the thermal effect [17], a model for elastocaloric cooling has to capture the full sample geometry. In the literature, various models for the pseudoelastic deformation of polycrystalline SMAs have been presented that differ in the length scale of interest, for instance the mesoscale (μm range) or the macroscopic (device) scale.

Micromechanical approaches resolve the evolution on a crystallographic (grain scale) level by constructing elastic, chemical and thermal energy contributions. Hence the typical grain sizes in TiNi films often being in the range below 1 μm restrict simulations to small representative volume elements in a hypothetically uniform sample [18,19]. Macroscale models as those related to the work of Tanaka and Nagaki, for instance, use an equation of state to calculate the internal phase fraction as a function of temperature and stress [20]. They achieve a good prediction of the macroscopic properties under uniaxial stress, but need to prescribe the transformation direction (M→A, A→M) for the whole sample [21]. On a mesoscopic length scale, the approaches related to Shaw & Kyriakides [15] present a 3D continuum-level description that captures the martensitic transition with a J_2 plasticity model, where front speed and number of bands are implicitly determined as part of the thermo-mechanical problem. Macroscopic stress-strain features and evolving band number have been determined during rate-dependent loading of 1D wires in Ref. [22], but the irreversible approach excluded unloading associated with self-cooling. An extension to the reverse M → A transformation for a 1D problem is presented in Ref. [23] using a free energy density with a strain gradient term, and a kinetic law. A 3D model with plastic flow rules including a local reorientation of the transformation strain tensor has been formulated by Azadi et al. [24] and applied to strain band evolution in TiNi stripes [25].

In SMAs, the austenite-martensite interfacial energy is a significant contribution, which is related to mechanical incompatibilities of the adjacent phases and leads to micro-elastic strains [26–28]. Phase-field (PF) models include this energy with a diffuse interface description that circumvents the singularities arising during nucleation, merging and vanishing of phase domains. At the scale of crystal grains, many PF models have been developed previously that use either the strain as order parameter with a Landau polynomial expansion for the free energy landscape [29], or a thermodynamic free energy and abstract order parameters (often a local phase fraction), e.g. Ref. [30]. Several PF models were introduced recently, that are able to capture transformation band formation in polycrystalline alloys. These models either reside in a 1D formulation applicable to wires [31,32] or are restricted to isothermal conditions for small tube [33] or stripe samples [34].

Here, we present a validated temperature-dependent PF model that allows the simulation of the load-dependent formation and evolution of strain and temperature bands in SMA films at the mesoscopic scale (~10 μm resolution). Therefore, limitations of previous PF models related to linear kinetics and small bulk driving forces, as formulated, for instance in Ref. [30], are circumvented. Due to the special interest in describing elastocaloric cooling applications, relatively high strain rates up to 0.1 s^{-1} will be explored.

2. Experimental methods

The materials under investigation are $Ti_{54.7}Ni_{30.7}Cu_{12.3}Co_{2.3}$ films that exhibit extremely high cyclic stability. Details on film fabrication and properties have been published recently [9,35–38]. The mechanical performance of the SMA films is investigated by uniaxial tensile tests. Stripe-shaped samples of 1.75 mm width and 15 mm length are obtained by a sacrificial layer etching process as described in Ref. [37]. The film samples are attached to alumina plates at both ends with two-component adhesive, which are then connected to the tensile test machine equipped with a 50 N force sensor. The resolution of force and displacement measurement is 0.25 N and 0.25 μm, respectively. Cyclic tensile tests are performed at different strain rates. Each cycle comprises a strain-controlled loading and unloading step, each followed by a halting step of 10 s for temperature equalization. Unloading is stopped at a small pre-load of 30 MPa in order to avoid buckling of the film. A maximum strain of 2.1%, closely below the onset of the linear elastic martensite regime, is chosen to increase sample lifetime. During tensile test experiments, the time-dependent surface temperature of the sample is monitored by an infrared (IR) camera with a spatial resolution of 25 μm and a field-of-view of 16 × 12 mm^2. Samples are covered with a thin layer of black carbon to increase emissivity. Simultaneously, a representative test area of 3 × 2 mm^2 is observed by a CCD camera. The local strain distribution is evaluated by digital image correlation (DIC) with a resolution of 80 μm.

3. Experimental results

3.1. Performance at the macroscale

The macroscopic stress-strain response of a TiNiCuCo film sample upon tensile load cycling is depicted in Fig. 1 for different strain rates. Engineering stress is determined by the measured force and initial cross section of the sample. The thermodynamic cycle comprises the following six stages:

(I.) In the first loading stage up to $\varepsilon \approx 0.6\%$ the material undergoes elastic deformation. The observed small deviation from linearity at the onset of the stress plateau can be attributed to a homogeneous transformation [8,39,40]. For instance, martensite fraction was found to reach 3% before strain localization sets in Ref. [41] and the amount of heat produced in this stage is typically very low [42].

(II.) The stress-induced A→M transformation starts in the second stage, which is associated with formation of local strain

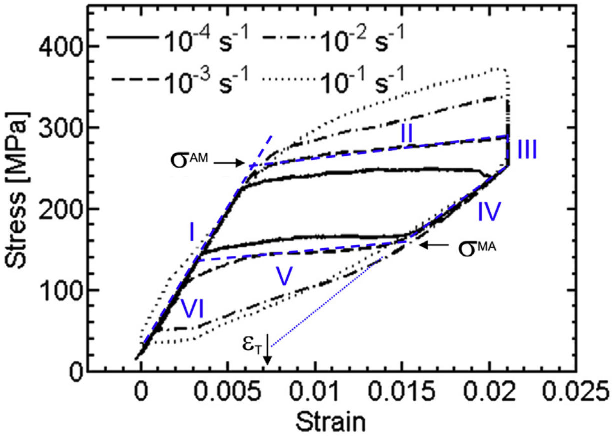

Fig. 1. Stress-strain characteristics of the TiNiCuCo film for different strain rates as indicated. The strain-controlled cycle comprises six distinguishable stages I - VI as indicated. Loading is stopped shortly before the end of the pseudoelastic plateau. The values of critical stress for austentite – martensite and reverse transformation σ^{AM} and σ^{MA}, respectively, are indicated for the strain rate of 10^{-3} s^{-1}.