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Thermomechanical discrete dislocation–transformation model of single-crystal shape memory alloy

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ABSTRACT

The interaction between martensitic phase transformation and plastic deformation affects the response of shape memory alloys (SMAs) during cyclic loading, in particular in terms of their pseudoelasticity characteristics and the shape memory effect. This interaction, which occurs at a sub-micron length scale inside single crystal grains, influences the reversibility and the actuation capacity of SMAs. In order to capture the sub-grain interactions while keeping the simulations tractable, a suitable modeling compromise between length scale resolution and computational effort is required. To this end, a model originally developed for multiphase steels assisted by transformation-induced plasticity is extended for shape memory alloys. Two new features, relevant for shape memory alloys, are introduced in the model, namely (i) the modeling of crystallographically reversible transformations and (ii) the thermal contribution in the free energy and the thermal effects on the transformation driving force. The two-dimensional model uses discrete dislocations to simulate plastic deformation due to slip and discrete regions to explicitly take into account the evolution of the martensitic phase. Through representative numerical simulations, the microscale coupling between phase transformation and plasticity is investigated with a view of elucidating (i) the effect of dislocations on the martensitic transformation, (ii) the effect of the phase transformation on dislocation slip and (iii) the interaction of both phenomena on the total reversibility of SMAs during cyclic loading. The results provide valuable information for the understanding of the interaction mechanism in shape memory alloys at the level of single crystals, which may be extended to an aggregate of grains.

1. Introduction

Shape memory alloys (SMAs) are able to regain an initial shape after an inelastic deformation upon applying appropriate thermal and/or mechanical cyclic loads. Depending on the external loading sequence, this particular behavior of SMAs is known as the “shape memory effect” or “pseudoelasticity”. In both cases, the underlying physical phenomenon that facilitates this behavior is a martensitic phase transformation.

The shape memory effect (SME) is a phenomenon where the material is cooled down to the martensitic phase from an initially austenitic phase. The cooling step is typically conducted without external mechanical load. Subsequently the material is mechanically deformed (nominally at constant temperature) and the external load is removed, leaving the material in a deformed state. The initial shape is recovered through a subsequent thermal loading step where the material transforms back to the austenitic phase.

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Pseudoelasticity, also referred to as "superelasticity", occurs when the material, initially in the austenitic phase, is mechanically loaded under (nominally) isothermal conditions and transforms into martensite. Removal of the load triggers a reverse transformation from martensite back to austenite and the specimen recovers its initial shape. Due to these properties, SMAs are employed in different applications such as actuators and sensors in aerospace, oil and gas, automation, and biomedical industries (Van Humbeeck, 1999; Hartl and Lagoudas, 2007).

A martensitic transformation is a displacive (diffusionless) solid-to-solid phase change between a higher symmetry parent phase (austenite) and a lower symmetry product phase (martensite). The martensitic transformation is crystallographically reversible since the atomic (lattice) structure of the austenitic phase is obtainable by heating up the martensitic phase. From a thermodynamical point of view, the transformation is irreversible since there is dissipation of energy in a thermomechanical cyclic process (hysteric behavior).

The inelastic deformation in a SMA typically occurs via the martensitic transformation, which generates the so-called "recoverable" strain (i.e., in addition to the elastic strain, the recoverable strain contains a contribution associated with the change in crystalline structure, the so-called transformation strain). However, an "irrecoverable" strain may also occur (see e.g., Hartl and Lagoudas, 2007), which affects the performance of SMAs upon repeated cyclic loading. Shape memory and pseudoelasticity tend to degrade after a few cycles, an issue that has been ascribed to the accumulation of plastic deformations (Olson and Cohen, 1975; Gall, 1999). This phenomenon under thermal cyclic loading is experimentally illustrated in Miller and Lagoudas (2000) and Ma et al. (2011). The irrecoverable strain is often due to the plastic deformation under thermal cycling when an external traction is prescribed (Hartl and Lagoudas, 2007; Dadda et al., 2008).

The coupling between phase transformation and plastic deformation is found in several types of metallic alloys and multiphase steels and is generically known as transformation-induced plasticity (TRIP). Ezaz et al. (2013) showed that the slip planes in the BCC-like structure of austenitic NiTi are active, indicating that both mechanisms (i.e., transformation and plasticity) may concurrently affect each other. The effect of TRIP in SMAs has been analyzed using a phenomenological model by Entchev and Lagoudas (2004). They found that the local stress fields associated with the martensitic transformation may trigger the activation of plasticity even when the external stresses are nominally lower than the yield stress of the material. At the sub-micron level (inside a single crystal grain) the phase transition from austenite to martensite typically occurs through the appearance of plate-like regions, often composed of twinned martensite. At a comparable length scale, plasticity is associated with the movement of dislocations along slip planes. Consequently, at the length scale of a single grain, the interaction between transformation and plasticity may be analyzed in terms of the effect that dislocations have on the nucleation and growth of the martensitic regions and, conversely, the effect that martensitic regions have on the generation and movement of dislocations. A somewhat open question is whether the dislocations assist the martensitic transformation (so called dislocation-induced transformation) (Fukuda et al., 1992; Ibarra et al., 2007) or they resist the growth of the martensite-austenite interface (Olson and Cohen, 1976). One objective of the present study is to provide a simulation-based insight on this interaction at the sub-micron level in the context of SMAs.

Discrete dislocation dynamic gives the opportunity to model the microstructure of plastic deformation by considering the nucleation, motion, and annihilation of dislocations (Amodeo and Ghoniem, 1990; Van der Giessen and Needleman, 1995). Shi et al. (2008, 2010) combined the discrete dislocation method with a proposed discrete transformation model to simulate the effect of phase transformation on plasticity in low-alloyed, multiphase TRIP steels. However their model is unable to predict reversible transformation in SMAs, and also it is unable to simulate the response of material under thermal loading. The two-way martensitic transformation and the thermal cyclic loading are the crucial elements to study the behavior of SMAs. Correspondingly, in this work, a modified discrete transformation model for SMAs is coupled with the discrete dislocation method to present a new discrete dislocation–transformation framework. This framework includes (i) the possibility of a crystallographically-reversible transformation and (ii) the effect of the thermal fields on the transformation behavior. Consequently, the model is capable of simulating the two-way shape memory behavior of SMA under thermomechanical loads. The model is applied in the present work to analyze the interaction between phase transformation and austenitic plasticity under cyclic thermal and mechanical loading for single crystal samples of SMA.

It is worth mentioning that, although the model does contain the required ingredients to study medium or high cycled loading, the simulations presented here are restricted to low cycling loading due to the computational limitations. Furthermore, as the focus of this work is to study the interaction between martensitic transformation and dislocation slip plasticity, the loading cases are limited to mechanical cycles (at constant nominal temperature) and thermal cycles (at constant nominal stress) from austenite to detwinned martensite. Despite these limitations, the model is capable of qualitatively predicting important changes in mesoscale properties of SMAs due to the effects of dislocations and martensitic nucleation and growth.

The structure of this paper is as follows: in Section 2, the discrete dislocation–transformation method for modeling the single-crystal behavior of shape memory alloys is presented. In Section 3 the isothermal pseudoelasticity of a sample is analyzed in detail for a single cycle and, subsequently, the accumulated effect of plastic deformation on the transformation behavior is studied in the context of multiple cycles. In Section 4, the two-way shape memory effect behavior, which corresponds to a full thermal cycle under an externally applied constant mechanical load, is investigated for distinct load levels. As for the isothermal case, the accumulated effect of multiple cycles is investigated. Concluding remarks are given in Section 5.