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Atomistic modeling of the orientation-dependent pseudoelasticity in NiTi: Tension, compression, and bending

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ABSTRACT

Pseudoelasticity in NiTi shape memory alloy single crystals depends on the loading direction. Here, we present a comprehensive study in which molecular dynamics simulations of austenitic bulk single crystals under strain-controlled tensile and compressive loading along the ⟨1 1 0⟩, ⟨1 1 1⟩, and ⟨1 0 0⟩ directions are performed, and the mechanical response of the crystals are contrasted. All simulations are performed using the MEAM interatomic potential proposed by Ko et al. (2015). The transformation strains and the Young's modulus of the initial austenitic and the final martensitic phases are compared with values obtained from the lattice deformation model and experimental results from the literature. Results show that depending on orientation the transformation occurs either through the formation of martensitic Lüders bands or through the transient formation of a multivariant martensite which, upon reorientation, becomes a dominant final single variant.

Simulations are also performed to assess the orientation-dependent behavior of nano-wires subjected to bending, since the flexibility of the wires is orientation dependent.

1. Introduction

A peculiarity of shape-memory alloy single crystals is their orientation-dependent pseudo-elastic behavior [2–5]. It is therefore crucial to be able to determine the best possible orientation for a specific application. Here, we perform molecular dynamics (MD) simulations of tensile and compressive loading of three differently-oriented austenitic nickel-titanium (NiTi) shape-memory alloys (SMAs) at 350 K and assess their performance. We also perform bending simulations of NiTi nano-wires in the same orientations to assess the orientation dependence of the bending behavior.

Equi-atomic NiTi SMAs are increasingly being considered for use in actuation and mechanical damping in nano- and micro- devices [4,6,5] due to their pseudo/super-elastic behavior. This feature stems from the ability of the alloy to exist in more than one phase depending on temperature and stress. Austenite is the high-temperature parent phase and has a cubic B2-type crystal structure. When an external load is applied at a high temperature, above the martensitic start temperature, the B2 phase transforms into the monoclinic B19′ martensitic phase, thereby accommodating deformations up to 10%. Upon removal of the external load, the material transforms back into the B2 phase and regains its initial shape manifesting its pseudo-elastic behavior.

This deformation behavior during a stress-induced martensitic transformation has been experimentally shown to depend on the orientation of the initial B2 crystal in micrometer size single-crystal specimens [7–11] and can be explained with the lattice deformation model (LDM) [12,13]. The final variant of martensite formed upon loading depends on the loading direction with respect to the initial B2 crystal, thereby causing a difference in the deformation behavior. Single-crystal SMA devices at the nano- and micro-scale can benefit from the higher transformation strains along certain orientations of the alloy. Since the direction-dependent behavior for a single crystal can be easily determined through simulations, atomistic simulation techniques such as molecular dynamics (MD) can be used to optimize the design of SMA devices by predicting the best orientation of the crystal for a given application. Prior to doing this, it becomes necessary to analyze and validate the SMA pseudo-elastic behavior under tension and compression predicted by MD simulations along various orientations.

The nano-structural changes and deformation behavior during pseudo-elasticity along certain orientations in bulk and nano-size specimens have been already shown through atomistic simulations by different groups and using different potentials; a complete picture with

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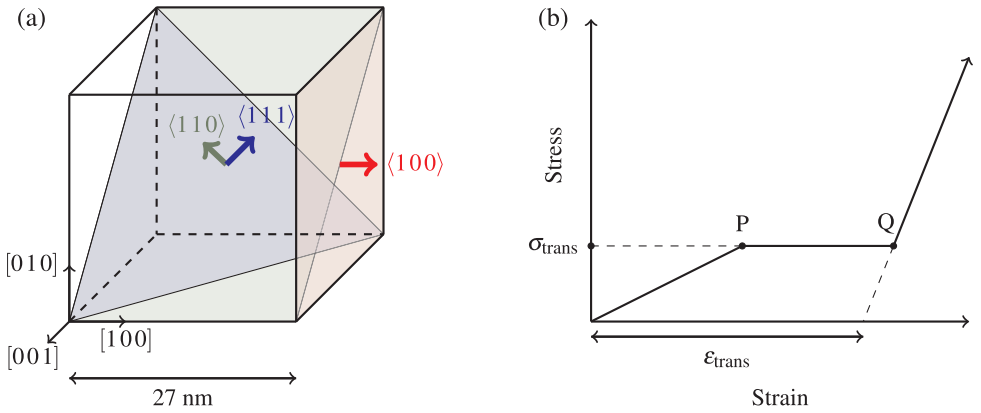

Fig. 1. (a) Schematic representation of the austenite crystal; the arrows indicate the different loading directions chosen for this study. (b) Representation of the typical austenitic-to-martensitic deformation behavior. The transformation strain and stress are indicated by ϵ_{trans} and σ_{trans}, respectively. Point P (Q) denotes the beginning (end) of the martensitic transformation.

the same system and potential is however missing and will be provided in this study. Zhong et al. [14] observed a reversible B2-B19′ transformation in 4.8 nm × 5 nm sized NiTi nano-pillars using the Finnis-Sinclair interatomic potential [15]. Their study was restricted to the compressive behavior of a ⟨1 1 0⟩ oriented B2 nano-pillar. Wang et al. [16] also used the Finnis-Sinclair potential to simulate cyclic compressive loading on ⟨1 1 0⟩ oriented nano-pillars and observed changes in the mechanical response with increasing cycles. More recently, Ko et al. [1] simulated the compressive stress-induced B2-B19′ transformation in a nano-pillar with a 10.7 nm × 10.7 nm cross-section. The pillar was loaded along the $\langle 0\,0\,1\rangle_{B2}$ direction at 450 K to validate their newly developed modified embedded atom method (MEAM) interatomic potential. Wang et al. [17] also performed similar simulations under adiabatic condition using the MEAM potential to study superelasticity under compressive loading along $\langle 0\,0\,1\rangle_{B2}$. In these works, the analysis has been restricted only to compressive loading along one orientation of the initial B2 phase. The MEAM potential has also been used to demonstrate phase transformation in NiTi polycrystals subjected to a single compressive [18] and cyclic compressive [19] loading. Recently, we have shown [20] that the MEAM potential [1] is more suited than the Finnis-Sinclair [21,14] to study pseudo-elasticity in single-crystal NiTi because of its ability to predict lattice and elastic constants more accurately. Hence, we use the MEAM potential to provide a comprehensive analysis of the elastic response of bulk NiTi under tensile and compressive loading before, during, and after phase transformation at different temperatures.

Three different initial orientations of bulk single-crystal austenite are considered in this contribution (Section 2) where tensile and compressive loading simulations are performed at 350 K. Results, shown in Section 3, indicate the directions along which the transformation strains are highest. The transformation strain values and the modulus of the initial and final phases are compared to experimentally known values and those obtained from the lattice deformation model [12,13]. The effect of temperature on the transformation behavior is examined by performing the same set of simulations at 400 K and 450 K. To determine the effect of the orientation dependence on an ideal actuator device, MD simulations of bending of nano-wires are also carried out and discussed in Section 4.

2. Methodology

MD simulations of the stress-induced martensitic transformation in NiTi are carried out using the MEAM interatomic potential [1]. The MEAM potential, which also takes angular interactions into account, captures the directionality in the metallic bonds more effectively than other potentials, making it the most suitable to predict phase transformation. The formulation of the MEAM potential and the parameters for NiTi can be found in the work of Ko et al. [1] and are not reported here. The potential predicts the martensitic start (M_s) and the austenitic finish (A_f) temperatures as 270 K and 490 K, respectively.

MD simulations of bulk NiTi are performed using LAMMPS [22] with the Nosé-Hoover [23] pressure and temperature control; the time integration is carried out using a velocity-Verlet algorithm [24] with a timestep of 0.5 fs. The initial structure is the ordered B2 phase, and three different loading directions are considered: ⟨1 1 0⟩, ⟨1 1 1⟩ and ⟨1 0 0⟩. Three periodic cubic simulation boxes, with faces normal to one of the loading directions are created and filled with atoms. Initially, an energy minimization run is performed using the conjugate gradient method to obtain the stress-free configuration of B2. Next, the simulation is run for 200,000 steps at zero stress and 350 K until the system is relaxed. This temperature is chosen since it is greater than the martensitic start temperature M_s, and B2 can therefore exist as the stable phase. Isothermal uniaxial displacement-controlled tension/compression is applied through a constant strain rate of $10^6\,s^{-1}$ along the loading direction. During loading, the average stresses over other surfaces are maintained at 0 MPa to allow for the simulation box shape and size to change. The deformation behavior is described by plotting the virial stress [25] on the x-plane in the x-direction against the corresponding engineering strain component. The size of the simulation box is increased in steps, and the above process is repeated for each box size until convergence of the stress-strain plot which is found to occur for a $27 \times 27 \times 27\ nm^3$ box. This size is therefore chosen as representative for bulk behavior and used to obtain the results discussed in the next section. A schematic representation of the initial system is shown in Fig. 1(a).

The mechanical behavior during a B2-B19′ phase transformation is characterised by the moduli of the initial B2 phase and the final B19′ phase and the corresponding transformation stresses and strains, as shown in Fig. 1(b). The stress at which the initial austenitic phase deviates from the initial linear elastic slope, denoted by point P in Fig. 1(b), is defined as the transformation stress σ_{trans}. The B2-B19′ transformation progresses until the entire crystal is converted to the martensitic phase (point Q in Fig. 1(b)) and continues with its elastic deformation. When the martensitic elastic loading part of the curve is extended to the horizontal axis (null stress level), the corresponding strain is defined as the transformation strain ϵ_{trans} at that particular temperature. The difference in stress-strain behavior in the phase transformation region during strain-controlled and stress-controlled loading was discussed in Ref. [20]. Here, we perform strain-controlled loading to study the nano-structural evolution during the B2-B19′ transformation. A stress plateau is not expected during the transformation because the transformation is neither instantaneous nor complete at the transformation strain. The uniaxial loading simulations are repeated at 400 K and 450 K where the stress-induced transformation