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Atomistic study on the super-elasticity of single crystal bulk NiTi shape memory alloy under adiabatic condition

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ABSTRACT

The temperature-induced phase transition and the super-elasticity (from the stress-induced phase transition) of equiatomic single crystal bulk NiTi shape memory alloys are investigated by the molecular dynamics method. By the simulation to the thermo-mechanical response of the single crystal NiTi alloy along the $\langle 0\,0\,1\rangle_{B2}$ under the compression/unloading and an adiabatic condition, the temperature change and the nucleation and growth of martensite transformation during the compression/unloading are discussed. The simulated results of molecular dynamics show that the single crystal bulk NiTi shape memory alloy exhibits a significant temperature change during the martensite transformation and its reverse under an adiabatic condition; moreover, a localized instability occurs apparently in the process of martensite transformation, which is closely related to the nucleation and growth rates of martensite phase; finally the effect of model size and strain rate on the thermo-mechanical response of the single crystal bulk NiTi alloy is also discussed, and no instability is observed in the simulated stress-strain curves if the model size is relatively larger, e.g., $8V_0$ and $13.824V_0$.

1. Introduction

Nearly equiatomic NiTi shape memory alloys (SMAs) are one of the most promising functional materials due to their super-elasticity, shape memory effect, good biocompatibility and wear resistance [1–4]. Super-elasticity means that the material undergoes a greater inelastic deformation, but can be spontaneously restored to its original shape after unloading [5,6]. Generally, nearly equiatomic NiTi SMAs can recover the strain up to 8% after unloading, while the recoverable strain of common metals is much less than 1.0% [7]. NiTi SMAs can experience a martensite transformation and its reverse, which is induced by applied stress (or strain), temperature and irradiation.

Molecular dynamics (MD) simulation had been often used to explore the microscopic deformation mechanisms of NiTi SMAs at the nanoscale. At present, the multi-body potential was widely adopted in the literature to describe the interaction of NiTi alloy atoms. Farkas et al. [8] proposed ternary Ni-Ti-Al potential based on the embedded-atom method (EAM) [9], but the proposed potential could not describe the phenomenon that B19′ phase was more stable than B2 one at low temperature. Lai and Liu [10] developed a NiTi potential by adopting the second-moment approximation of the tight-binding theory [11,12], and then better described the phase transition between austenite and martensite phases. Mutter and Nielaba [13] and Zhong et al. [14] modified the potential function developed by Lai and Liu [10] to ensure the smooth cutoff behavior of this potential. Ren and Sehitoglu [15] developed a semiempirical potential with Finnis–Sinclair formalism [16,17] and investigated the martensitic transformation of NiTi alloy. In addition, a modified embedded-atom method (MEAM) [18–21] was adopted by Ishida et al. [22], Saitoh et al. [23] and Chun et al. [24] to fit the interatomic potential of NiTi alloy. Recently, Ko et al. [25,26] and Muralles et al. [27] fitted the NiTi SMA potential using the second nearest-neighbor (2NN) MEAM potential [28–30], and then well described the temperature- and stress-induced phase transitions.

However, existing MD simulations of NiTi SMAs mainly focused on the effects of the loading rate, ambient temperature [5–7,26,31,32], cyclic deformation [26,33], grain size and precipitate phase [26,34] on their super-elasticity. For examples, Sato et al. [5] found that the relationship between the stress and the volume

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fraction of martensite phase did not depend on the strain rate; Zhong et al. [6] concluded that an irreversible twinning occurred owing to the dislocation pinning of twin boundaries by performing the MD simulations with different peak strains and at different temperatures; Yin et al. [7] investigated the effects of temperature and strain rate on the phase transition of NiTi SMAs under the uniaxial compression, and suggested that the interaction between the phase transition and plastic deformation leaded to different crystal structures after loading; Chowdhury et al. [31] demonstrated the temperature dependence of the stress-strain curves for NiTi SMAs under the tension and compression along the $\langle 0\,1\,1\rangle_{B2}$, Ko et al. [26] also revealed that polycrystalline NiTi SMAs exhibited a strong dependence of the martensite transformation stresses on the applied strain rate; Mirzaeifar et al. [32] studied the phase transition of NiTi nanowires driven by temperature and stress, and found that the tendency to reduce the surface energy in the NiTi nanowires could lead to the phase transition from the austenitic B2 to the martensitic B19 phase.

Cyclic deformation and associated damage evolution have significant influences on the assessment to the reliability and service-life of NiTi SMA devices. Ko et al. [26] revealed that the pre-training by cyclic loading could greatly reduce the irrecoverable strain; also they reproduced the temperature- and stress-induced phase transitions observed in the experiments by using a polycrystalline model without internal defects, and then proposed a strain contribution mechanism (rather than the internal defect contribution mechanism) and successfully explained the asymmetric nucleation and growth occurred in the martensite transformation and its reverse of nano-crystalline NiTi SMAs. Wang et al. [33] found that dislocation slipping and twinning were responsible for the changes in the atomic structure and mechanical responses such as the accumulated irreversible strain and the degeneration of super-elasticity occurred during the cyclic compression-unloading. It is well-known that the super-elasticity of NiTi SMAs exhibits a significant thermo-mechanical coupled interaction. Temperature change caused by the latent heat of phase transition and mechanical dissipation is the physical nature of rate-dependent super-elasticity of NiTi SMAs [35,36]. However, it should be noted that the existing MD simulations of NiTi SMAs do not pay attention to the temperature change during the inelastic deformation, and the effect of the internal heat generation (originating from the transformation latent heat and mechanical dissipation) on the thermo-mechanical coupled response of NiTi SMAs has not been discussed yet by MD method.

Considering the requirements of ensemble environment in MD simulation, the MD simulations of single crystal bulk NiTi SMA under an adiabatic condition are performed in this work to reflect the temperature change occurred during the repeated phase transition, and the energy required for the increase of system temperature during the phase transition is analyzed. Then, the nucleation and growth of martensite phase and localized instability occurred in the process of phase transition are addressed without considering the effect of grain boundary, but considering the effect of model size. A novel analysis strategy on the thermo-mechanical coupled stress-strain response of NiTi SMAs by using the MD method at nano-scale is provided.

2. MD model

In this work, the simulation cell which consists of 50 at.% Ni and 50 at.% Ti atoms is established, as shown in Fig. 1a. A simulation cell with the size of 106.63 Å × 106.63 Å × 105.56 Å, which consists of 87,500 atoms, is constructed, and is defined as a model size of V_0. The simulation cell consists initially of the ordered B2 austenite phase, as shown in Fig. 1b and c. The lattice constant a_0 of the initial unit cell is 3.016 Å [25]. According to Chowdhury et al. [34,37,38], the simulation cell for the bulk material can be established by applying periodic boundary conditions on the crystal facets. In the process of relaxation, the system temperature and pressure are controlled at a set temperature and zero stress state. The time step used in the simulation is set as 0.002 ps. The temperature and pressure damping parameters are 0.2 and 2.0, respectively.

In the MD simulation, the NiTi atomic interaction potential developed by Ko et al. [25] is adopted to describe the interactions among the atoms of Ni-Ni, Ti-Ti and Ni-Ti. It is confirmed that the NiTi potential developed by Ko et al. [25] can be successfully applied to study the temperature- and stress-induced phase transitions of NiTi SMAs [25–27].

As shown in Fig. 1a and d, a compression-unloading is applied to the single crystal bulk NiTi SMA along the $\langle 0\,0\,1\rangle_{B2}$ under a strain-controlled loading and unloading condition and at an identical strain rate during the loading and unloading, and the stresses along the *X* and *Y*-directions are kept to be zero. More details about the simulation method and the expansions of materials during uniaxial deformation can be referred to Ko et al. [25,26] and Muralles et al. [27]. In an adiabatic case, since the periodic boundary conditions are applied along all three directions of bulk NiTi SMA, any isothermal or isometric ensemble (such as micro-canonical, canonical and isobaric-isothermal ones) cannot be used [39]. Therefore, an isobaric-isenthalpic ensemble (NPH) is selected to investigate the stress-induced phase transition (i.e., super-elasticity) of single crystal bulk NiTi SMA under the adiabatic condition in this work. The NPH ensemble can be used in a non-equilibrium MD simulation so that the system can be kept being under an adiabatic condition [39]. All the temperature changes in the single crystal bulk NiTi SMA are counted during the compression-unloading.

It is indispensable to adopt a suitable method to describe the phase transition degree of NiTi SMAs in the process of loading/unloading. Zhong et al. [6,14] characterized the phase transition by an order parameter which was defined as the sum of all the shear components in the simulation cell. By analyzing the nearest neighbor environment of the austenite B2 and martensite B19′ phases, Mutter and Nielaba [13,40,41] and Qin et al. [42] employed the nearest neighbor distances of each atom to construct the order parameter. Sato et al. [5], Saitoh et al. [23], Mirzaeifar et al. [32] and Wang et al. [33] compared the axes or angles inside the unit cell with reference phases so that the phase transition can be detected. Yin et al. [7], Ko et al. [26] and Wang et al. [33] distinguished the B2 austenite and B19′ martensite phases by using the common neighbor analysis (CNA) [43–46]. In addition, the radial distribution function was also used to evaluate the phase transition [13].

Among the analysis methods of phase transition, the CNA method can be used to characterize the structural state of each unit cell real-timely [33]. The CNA method computes a characteristic signature from the topology of bonds that connect the surrounding neighbor atoms [46]. The cutoff distance for the presumed crystal structure is chosen to determine the appropriate nearest neighbors of an atom and identify the local crystal structure around an atom. The CNA method can recognize five crystal structures with a specific cutoff distance in LAMMPS, i.e., 1 for FCC, 2 for HCP, 3 for BCC, 4 for icosahedral and 5 for the rest crystal structures [47]. Since B2 austenite phase is a body centered cubic (BCC) crystal structure, it is represented by 3. Similarly, since B19′ martensite phase is a monoclinic crystal structure, by neglecting the effect of unit cells with imperfect surface in the initial model, it can be classified as the one belonging to the rest crystal structures during the phase transition and its reverse and then is represented by 5. It has been confirmed that such a treatment is very suitable for distinguishing the B2 austenite and B19′ martensite phases and assessing the