Computational Materials Science 146 (2018) 61–69

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Molecular dynamics simulation on the shape memory effect and superelasticity in NiTi shape memory alloy

Xiang Chen [a], Teng Liu [b], Rui Li [b,*], Jiushan Liu [b], Yang Zhao [a]

[a] School of Advanced Manufacturing Engineering, Chongqing University of Posts and Telecommunications, Chongqing 400065, China
[b] School of Automation, Chongqing University of Posts and Telecommunications, Chongqing 400065, China

ARTICLE INFO

Article history:
Received 10 October 2017
Received in revised form 9 January 2018
Accepted 9 January 2018

Keywords:
Shape memory alloy
Molecular dynamics simulation
Shape memory effect
Superelasticity

ABSTRACT

Molecular dynamics (MD) simulations Ni-Ti based on a second nearest neighbor modified embedded-atom method potential were performed to study atomic-scale mechanical behavior and microstructural evolution of Ni-Ti alloy at different temperatures. By using four calculated characteristic transformation temperatures, the optimum simulated temperature ranges were determined. At temperatures lower than M_s, a thermally induced self-accommodating martensitic phase consisting of three variants formed. Each of the two variants was twin structures. In the subsequent loading process, the most favorable variant grew with the movement of interfaces among the variants, which produced remnants of the residual strain after unloading. After heating up to over A_f, the residual strain disappeared and the shape recovered to the original. The shape memory effect under austenite state was also performed, wherein the sample exhibited a typical stress–strain temperature curve and remained in a martensitic state after unloading. After heating at a high temperature, the martensite transformed back into its parent phase accompanied with the recovery of residual strain. The material exhibited superelastic behavior above A_f, and the critical transformation stress increased with increased temperature. Some parts of B2 structures remained at the end of the plateau stage and continued transforming into martensites during the hardening stage for both $T > A_f$ and $M_s < T < A_f$. The critical stresses for transformation satisfied the Clausius–Clapeyron relationship at $T > M_s$.

1. Introduction

Recently, the Ni-Ti shape memory alloy (SMA) has received increasing attention because of its unique shape memory effect (SME) and pseudoelasticity (or superelasticity), which makes it widely used in aerospace, mechanical electronics, transportation, biomedicine, and automotive industries [1–3]. Previous studies indicated that these unique properties result from the temperature- or stress-induced reversible martensitic phase transformation [4]. There are four characteristic phase transformation temperatures: martensite transformation start temperature M_s, martensite transformation finish temperature M_f, austenite transformation start temperature A_s and austenite transformation finish temperature A_f. In general, Ni-Ti SMA presents B2 crystal structure (austenite) at high temperature and exhibits superelastic characteristics, whereas cooling below M_s generates monoclinal B19' crystal structure (martensite) and exhibits pseudoelasticity [5].

Because of the rapid growth of Ni-Ti alloys in various fields, scholars have made abundant studies on the thermal-mechanical properties of Ni-Ti, both in micro and macro experimental aspects [6–14]. Under uniaxial compression loading, it was found that temperature has a great influence on the stress–strain curves by Ng and Sun [6]. When the temperature is above A_f, the critical stress required for martensitic transformation increases with the increase of temperature [6]. The shape memory effect and the pseudoelasticity under austenite state were investigated by Miyazaki et al. [7]. They found that when the temperature ranges from M_f to A_s, the austenites change into martensites and remain under martensitic state after unloading. When heated to a high temperature, the martensites then transform back into austenites, and the residual strain recovers [7]. On micro-scale, Li et al. [8] found that while under stress loading, Ni-Ti alloy mainly undergoes martensitic reorientation at low temperatures much lower than M_f. Although the mechanical properties of Ni-Ti SMA on macro- and micro-scale were experimentally studied in detail, the microstructure evolution of the martensite phase transformation under stress- or thermal-induced was scarce, and it is still difficult to directly

* Corresponding author.
E-mail address: lirui_cqu@163.com (R. Li).

https://doi.org/10.1016/j.commatsci.2018.01.026
0927-0256/

observe the micro-mechanism of the martensitic phase transition process via experimental methods.

Molecular dynamic (MD) simulations have been widely used to study the martensitic phase transformation of Ni-Ti alloy from an atomic scale, and it is of great significance to study the microscopic mechanism of phase transition or martensitic reorientation in order to better apply this smart material [15–18]. Lai and Liu [19] firstly proposed the embedded-atom method Finnis-Sinclair (EAM-FS) potential to describe the atomic interaction of Ni-Ti alloy, which was modified by Zhu et al. [20,21] to study the martensite phase transformation of Ni-Ti alloy. Mutter and Nielaba [22] also improved Lai's potential and simulated the effects of temperature on the stress-induced martensite phase transformation. Ko et al. [23] optimized a Ni-Ti potential based on the second nearest neighbor modified embedded-atom method (2NN MEAM), and accurately reproduced the temperature- and stress-induced phase transformation in equiatomic Ni-Ti alloy. Srinivasan et al. [24] compared the 2NN-MEAM potential with the EAM-FS potential in detail and found that the 2NN-MEAM potential can calculate the crystal constant, and predict martensite phase transformation more accurately.

Recently, scholars mainly studied the pseudoelasticity or SME of Ni-Ti alloy with the EAM-FS potential [16,17,19–22]. The detail of temperature-induced and stress-induced phase transition of Ni-Ti alloy with a 2NN-MEAM potential were rarely reported [15,23]. Most literatures discuss the pseudoelasticity of Ni-Ti alloy, while the uniaxial compression behavior at the state of martensite phase was referred rarely. In present research, authors used the molecular dynamic method based on a 2NN-MEAM potential optimized by Ko et al. [23] to simulate temperature- and stress-induced martensitic transformation at different temperatures. The characteristic temperatures were calculated. According to the martensite transformation temperatures, the simulated temperature is divided into three ranges: (1) at T < Ms, where martensitic reorientation and shape memory effect under martensitic state were discussed; (2) at Ms < T < Af, where the study was centered on shape memory effect under austenitic state; and (3) at T > Af, where superelasticity was investigated.

2. Method and model

2.1. Interatomic potentials

Uniaxial compression of Ni-Ti alloy has been carried out by using large-scale atomic parallel computing software (LAMMPS) [24]. It is widely believed that the most important aspect of MD simulation is the selection of appropriate interaction potential between atoms. The 2NN-MEAM potential [23] was used to study the thermal-induced phase transformation and uniaxial compression behavior of Ni-Ti alloy in nanoscale. The specific coefficients of the 2NN-MEAM between Ni-Ni and Ti-Ti were improved by Lee et al. [25] and Kim et al. [26], as listed in Table 1. Detailed parameters of the interaction potential of Ni-Ti were optimized by Ko et al. [23], which are summarized in Table 2.

2.2. Model

The model schematic diagram is shown in Fig. 1(a). The three-dimensional size of the [0 0 1] crystal orientation is 39a (a is the lattice constant). The x, y, and z axes correspond to [1 0 0], [0 1 0], and [0 0 1] crystal orientations, respectively. Periodic boundary conditions are adopted in all three directions. The sample was initially equilibrated under B2 structure, then transforming into the B19' structure after temperature or stress was applied. The phase transition schematic diagram between B2 phase and B19' phase is shown in Fig. 1(b).

The constant integral time step in all simulations was 1 fs. The temperature and pressure control were adopted by the isobaric-isothermal (NPT) ensemble and the Parrinello-Rahman barostat was used to relax the box in the stage of thermal-induced martensite transformation. Before applying stress, each atom obtained a suitable initial velocity. The initial model was relaxed for 20 *ps* under the NPT ensemble to make the temperature and pressure achieve a dynamic balance. The uniaxial compression was then carried out along the x-axis. The stress was gradually loaded up to 2.1 GPa and unloaded to 0 GPa, with loading and unloading rates of ±0.021 GPa/ps. The above simulation was carried out at different temperatures to discuss the effect of deformation temperature on phase transition. If the residual strain generates after unloading, the samples will be heated to 550 K with a rate of 1 K/ps to study the shape memory effect. The simulation results were visualized by OVITO program [27]. In order to make the phase transition atomic structural evolution more clearly, the CNA algorithm [28] and the polyhedral template matching (PTM) [29] were used to differentiate the B2 austenite and B19' martensite phase.

3. Results and discussion

3.1. Temperature-induced transformation

Stress-induced martensitic transformation of Ni-Ti alloy is affected strongly by the deformation temperature (T). Thus, the characteristic phase transformation temperatures should be identified. For this purpose, a cooling and heating process is performed on the Ni-Ti sample. Firstly, a B2 structured Ni-Ti atomic model is established at 500 K, then the temperature will be gradually decreased to 100 K. It will then be increased to 600 K, with cooling and heating rates of ±0.5 K/ps. The change of the atomic volume against temperature during the cooling and heating process is shown in Fig. 2. The evolution of microstructures (B2 and B19') within the material is also inserted**.** In previous studies [23,30], a sharp increase of the atomic volume predicts the austenite transformed into B19' phase. During the cooling process, the B2 phase starts to transform into B19' at 235 K, which is considered as the start temperature of forward martensite transformation (M_s). The martensite finish temperature (M_f) is about 229 K. After cooling to 100 K, the martensite can be observed clearly in the (1 0 0) surface. The inclination angle of the box is nearly 95°65', whereas some discontinuous stacking faults were formed within the martensite variant, as shown in yellow[1] lines in Fig. 2. A similar structure of martensite variant was also obtained in Ni-Al shape memory alloy via MD simulation [31]. While heating to 434 K (corresponding to A_s), the atomic volume decreases rapidly which implies that the martensitic phase starts to recover back into the B2 structure. When the temperature reaches 441 K (corresponding to A_f), the reverse martensite transition finishes and the atomic structure comes back to the B2 structure, whereas the box becomes cube again. Based on these results, three simulated temperature sections $T < M_s$, $M_s < T < A_f$, and $T > A_f$ are identified.

3.2. Shape memory effect

There are two cases of shape memory effect depending upon the deformation temperature. When the temperature is below or equal to M_f, the material is completely composed of martensite. In this case, the strain is the deformation of martensite. On the

[1] For interpretation of color in Fig. 3, the reader is referred to the web version of this article.