



Atomistic simulation of shape memory effect (SME) and superelasticity (SE) in nano-porous NiTi shape memory alloy (SMA)

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ARTICLE INFO

Keywords:

Atomistic simulation
Shape memory effect
Superelasticity
NiTi shape memory alloy
Nanoscale
Porosity

ABSTRACT

Porosity can play an important role in altering the phase transformation characteristics of NiTi shape memory alloys (SMA), thus changing its shape memory as well as its superelasticity properties. This work, based on atomistic simulations of binary NiTi SMA, documents the effects of porosity at the nanometer length scale on phase fraction evolution kinetics, transformation temperatures, and stress-strain response. Classical molecular dynamics simulations are performed using a well-examined and verified Finnis-Sinclair type embedded-atom method interatomic potential. Simulation results for the nano-porous NiTi with various porosity configurations are compared to non-porous NiTi. The martensite phase fraction and transformation temperatures increase noticeably with increasing porosity, and the stress-strain response shows noticeable variation with porosity. The residual strain and hysteretic energy dissipation capacity increase significantly with increasing porosity.

1. Introduction

Important properties of NiTi shape memory alloy (SMA) emanating from the temperature and stress or strain induced displacive phase transformation process are the shape memory effect (SME) and superelasticity (SE). While the SME relates to the thermally induced phase transformation process, the SE relates to the stress or strain-controlled phase transformation process at different temperatures. Because of its tunable and well characterized material properties, NiTi SMA has become one of the alternative and attractive choice for research as well as for industrial applications. Review papers [1–3] and other recent studies [4–7] report investigations on novel smart components and devices at various length scales, from nanometer to continuum, using NiTi SMAs and/or relevant composites. The SME and SE properties can be altered and/or tuned through tailoring the evolution of microstructure, i.e., the evolution kinetics of different phases and this leads to a broader spectrum of applications of NiTi SMA.

Microstructure of NiTi SMA can be tailored via for example altering its composition or by the introduction of free surfaces/interfaces through porosity. Based on previous studies [5–10], tailoring the microstructure can alter the: (i) evolution and growth/nucleation kinetics of different phases; (ii) phase transformation temperatures and the stress/strain response. Different studies show that changing the Ni/Ti fraction, and/or adding other elements (such as in ternary Ni–Ti–X (X = Cr, Cu, Hf, Pd, V, Zr) and quaternary Ni–Ti–Cu–Y (Y = Co, Pd)

SMAs, etc.) can significantly alter the phase transformation temperatures, critical energy or stress required for phase transformation, and the width of the thermal and/or stress hysteresis. Recent studies by the authors and others at the nanometer length scale [4–10] demonstrate the significant effect of free surfaces and interfaces on the phase fraction evolution, transformation temperatures and stress-strain response. Increase in available surface area supports some unique behavior in the phase transformation process [4–10], which may not present in non-porous NiTi. Similarly, porosity is an alternative way to tailor the microstructure evolution process, and thereby altering the SME and SE properties of NiTi SMA.

Porous SMAs, the most common one being NiTi, have been studied extensively, starting in the 1980s with applications in the area of biomedical engineering. Production methods for porous NiTi vary widely, yet the basic processes fall under the general category of powder metallurgy. The extensive literature in this area, including physical testing and characterization of porous NiTi can be traced through a recent review [11]. In parallel, extensive efforts on modeling the thermo-mechanical behavior of SMAs in general and NiTi in particular have also been undertaken. Unit cell and spatial averaging modeling methods (based on mean field method for homogenization or micro-mechanical averaging method) [12–16] yield effective macroscopic constitutive relations including the evolution of phase fractions in the SMA. Also, the effects of hydrostatic pressure, asymmetry of the constitutive response between tension and compression, are included in the

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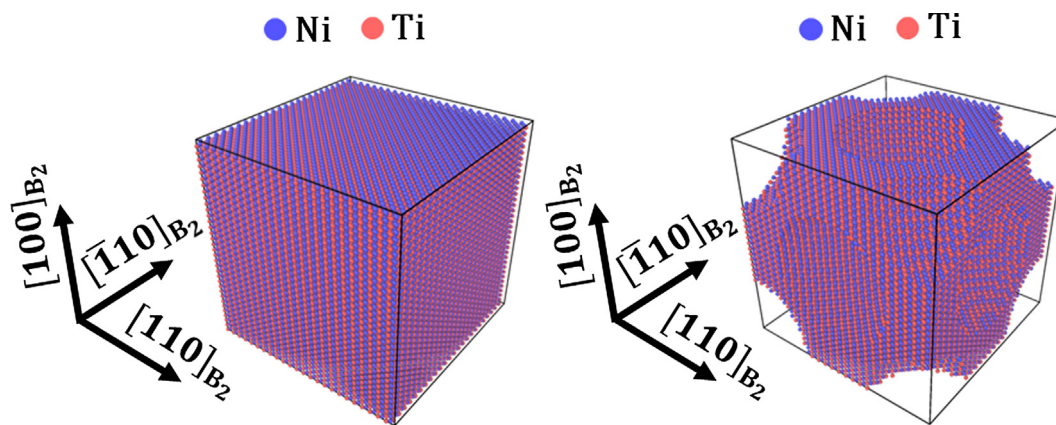


Fig. 1. MD simulation cell corresponding to (a) non-porous NiTi and (b) porous NiTi. Periodic boundaries are imposed ensuring that the pores at the cell-boundaries are continuous.

model presented in [17]. Numerical modeling of SMAs, based on the phenomenological constitutive relation are reported in the literature [18–23]. Other mesoscopic/microscopic models for porous NiTi include those reported in [24,25], and some of them are developed from phase-field theory [26,27]. Significant level of experimental studies [28–31] are also reported that explore the phase transformation and super-elasticity property of SMA, under a wide range of constant and gradient porosity.

From numerous studies it has been observed that the key to the behavior of NiTi, and thus of porous NiTi, is its phase transformation kinetics, and such kinetics depend on spatial scale [9,10]. It has been observed from previous studies [4,7–10] that, at the nanoscale, the presence of free surfaces, substantially alters the phase transformation kinetics of NiTi. Free surfaces act as defects that initiate the forward and reverse phase-transformation process involving the different variants of the martensite phase and the austenite phase respectively. However, such kinetics, and their effects on the SME and SE of porous NiTi, have not been studied at the nanometric scale, and this creates a gap of knowledge about the behavior of porous SMAs, at the nanometer length scale. Thus, this study addresses the nanoscale porous NiTi, of various porosity configurations, computationally, and compares the results to available experimental data.

Specifically, the present study addresses the effects of porosity on the SME and SE behavior of NiTi SMA. Porous NiTi cells of various levels of porosity are simulated using an interatomic potential that is has been well-documented for its effectiveness in simulating NiTi SMA. The effects of porosity on the temperature and stress/strain induced phase transformation process is reported in terms of martensite phase fraction, transformation temperatures, and width of the thermal hysteresis. Also, the effects of porosity on the stress-strain response, residual strain and hysteresis energy dissipation capacity of NiTi SMA at various temperatures are reported.

2. Methods

This section provides the information about the interatomic potential, MD simulation process in LAMMPS [32,33] and on the characterization techniques used to separate the spatial domain of austenite phase from that of martensite. A brief description of the simulation methods is given since they are well-established and described in details in the literature [9,10,34].

2.1. Interatomic potential

In the present study, a well-established many-body Finnis-Sinclair type interatomic potential (as referred by the embedded-atom method (EAM) in literature) for the binary NiTi alloy is used. The EAM potential

was originally developed by Lai and Liu [35] considering the second-moment approximation of tight-binding theory (TBSMA); and later improved by Zhong et al. [6,36,37] through adding a smooth cutoff behavior (to avoid the diverging forces during simulation, due to large atomic displacements) above a critical interatomic distance [6,36,37]. Different parameters of this EMA potential are estimated by fitting the properties (obtained from first principles calculations) of the B2 phase at 0 K, with the potential cut off radius $r_c = 4.2 \text{ \AA}$ [6,36,37]. It has been shown in several studies [6,7,9,10,34,36,37] that this modified potential provides accurate values of the lattice constants and energies of different phases of NiTi, when compared to those obtained from ab-initio calculations [36,37]. Further, other studies confirm that this modified potential predicts appropriately (i) the phase transformation (PT) process due to the temperature i.e. shape memory effect (SME) and super-elasticity (SE) [4,7–10,36,37], (ii) transformation temperatures and stress values [4,6,8,9,34,36,37], and the phase fraction evolution kinetics and the stress-strain responses [4,6,8,9,34,37]. Since this potential is well documented in the literature [6,7,9,10,34,36,37], further details are not provided here; rather, a brief description is provided in the [supplementary material](#).

2.2. MD simulation process

In this study both the shape memory effect (SME) and super-elasticity (SE) aspects of nano-porous NiTi are explored computationally and the results are compared to non-porous ones. In all MD simulations, the initial MD cell size is $250 \text{ \AA} \times 250 \text{ \AA} \times 250 \text{ \AA}$, with periodic boundary conditions in all three directions.

To generate porous MD simulation cells, a MD visualization and rendering software - OVITO [38] is used. Fig. 1(a) shows a typical MD simulation cell corresponding to a nonporous B2 NiTi system as rendered using OVITO. To generate porous MD cells, spherical domains of different diameters (ranging from $10 \text{ \AA}$ to $50 \text{ \AA}$) are identified within the non-porous structure (using OVITO), and equal number of Ni and Ti atoms are removed from within this sphere.

For all simulations, the pristine simulation cells are initially geometrically optimized through the stress-controlled conjugate gradient energy minimization method. At each temperature of interest, the system is initially subjected to NPT (i.e. constant pressure = 0 GPa) conditions for 360 ps, where the shape and size of the simulation boxes are allowed to change to ensure that both pressure as well as the individual components of the symmetric stress tensor are set to zero. This is followed by constant volume (NVT) conditions for an additional 240 ps. In each case of NPT or NVT stabilization, the adopted time step is $\Delta t = 0.0005 \text{ ps}$. During the simulation process, the temperature and pressure is controlled by a Nose-Hoover thermostat and barostat. In order to remove the effects of thermal fluctuations while analyzing

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