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# Origin of low thermal hysteresis in shape memory alloy ultrathin films



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## ARTICLE INFO

### Article history:

Received 16 October 2015

Accepted 21 October 2015

Available online xxx

### Keywords:

Size effect

Martensitic transformation

Shape memory alloys

Hysteresis

## ABSTRACT

Hysteresis in martensitic transformations (MT) limits the usefulness of shape memory alloys (SMAs) in nanosized devices that require high sensitivity, high durability and high energy efficiency. Previous studies have shown that the MT is hindered in the surface region of nanosized SMAs, and therefore there is little hysteresis. However, we find that the hysteretic behavior in SMA nanofilms is not related to the MT suppression. Rather, the decrease in hysteresis is due to weaker spontaneous lattice distortion and spatial heterogeneity, leading to a more continuous phase transformation process. We demonstrate this by designing two classes of nano-sized SMAs, a free-standing  $\text{Ni}_{62.5}\text{Al}_{37.5}$  film in which the surface region promotes MT, and a multilayer of  $\text{Fe-Ni}_{62.5}\text{Al}_{37.5}\text{-Fe}$  in which the interface region suppresses MT. Both cases show a decrease in hysteresis with decreasing film thickness. Our findings suggest a method to reduce hysteresis in conventional bulk SMAs.

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## 1. Introduction

A martensitic transformation (MT) enables shape memory alloys (SMAs) to exhibit fascinating properties such as shape memory effect and superelasticity. Based on their unique properties, SMAs have been widely used in sensors, actuators, medical devices, and other applications [1–3]. However, special attention needs to be given to the phenomena of complex hysteresis associated with lack of reversibility under loading due to the application of strain/stress control. This can lead to a reduction in the performance of devices [4–7]. This hysteretic phenomenon is also encountered in many other smart material actuators that involve magnetic materials or piezoelectric materials [8–10]. Therefore, in order to improve the position control accuracy of an SMA actuator, it is necessary to reduce the effects of hysteresis.

It has been shown that reducing the size of SMAs down to the nanoscale (such as SMA nanoparticles, SMA nanocrystallines) can decrease significantly the width of the martensitic transformation hysteresis loop [11–17]. Many theoretical models of martensitic transformations have been developed to explain the small hysteresis in nanosized SMAs, and the one that has performed well is the core–shell model [18–20]. For example, Zhang et al. studied

freestanding SMA nanoparticles and showed that the surface region suppressing the B2–B19 transformation locally plays a dominant role in the size dependent transformation behavior, leading to nonhysteretic superelasticity [12,19]. Sun et al. subsequently used this model to explain the small hysteresis in TiNi nanocrystals [21,22]. Nevertheless, experimental results in other phase transforming systems, such as ferroelectric nanofilms, have shown that the surface region can suppress the spontaneous transformation in a number of cases but can promote phase transformation in others [23–25]. Thus, the open questions are (1) what is the hysteresis behavior in the case where the effects of the surface promotes phase transformation? (2) Is the reduction in transformation hysteresis related to the phase transformation occurring in the near-surface region? These two questions and their relationship are still not clear.

In this work, we study the thermal induced phase transformations in nanosized SMAs, aimed at achieving an atomic-level understanding of the hysteresis behavior. The basic idea is as follows: the transformation temperature can be influenced by the surface/interface effect, and we can design two types of ultrathin SMA films (i.e., one with increased transformation temperatures in thin films, the other with decreased transformation temperature) by engineering the surface/interface energies, and then comparing the hysteretic behavior in the two cases. We first use molecular dynamics (MD) simulations to find the relationship between the surface/interface energy and the size dependent characteristic temperatures of the MT. The thermal hysteresis during the

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martensitic transformation in both cases is then calculated to investigate its relationship to the surface/interface effect. Finally, we discuss the main contributions to the hysteresis behavior in nanosized SMAs.

## 2. Methodology

The ultrathin SMA film model under investigation is created in a model SMA (e.g.  $\text{Ni}_{62.5}\text{Al}_{37.5}$ ) monolayer or model SMA/non-transformed metal (e.g.  $\text{Ni}_{62.5}\text{Al}_{37.5}/\text{Fe}$ ) multilayer. The samples are oriented by stacking {110} NiAl atomic planes along the y axis, with the interfaces located parallel to the x-z plane, as shown in the inset of Fig. 1(a). Periodic boundary conditions are applied in the x and z directions while the thickness direction is bounded by two free surfaces. The periodic x and z dimensions are 23.98 nm and 33.75 nm, respectively. In order to study the influence of SMA layer thickness on the phase transformations several different thicknesses from 3 nm to 20 nm were selected. We adopted an embedded atom method (EAM) interatomic potential developed by Dudarev and Derlet for Fe [26]. A semi-empirical interatomic potential of the form proposed in Ref. [27] by Farkas et al. is used to describe the B2-orthorhombic phase transformation in  $\text{Ni}_{62.5}\text{Al}_{37.5}$ . The interaction potentials of Fe and Al/Ni were based on the usual form used for other metal pairs [28]. These potentials have produced good results for phase transition and defect formation energies [19,27,29], however, one should not expect that such semiempirical potentials can reproduce the detailed properties of a specific SMA or material system.

The initial samples were relaxed by quenching with the conjugate gradient algorithm. The samples were then annealed at 1000 K, above the NiAl parent phase stabilizing temperature, for at least 120 ps by using a Nose-Hoover thermostat [30] and Parrinello–Rahman barostat [31] within the isothermal-isobaric ensemble. After this procedure, we performed MD simulations of cooling and heating on the annealed samples utilizing the LAMMPS code [32]. The cooling and heating processes involve cyclic increase or decrease in temperature with rates of 0.01 K/ps.

## 3. Results and discussion

### 3.1. Thermodynamic model of martensitic transformation in nanosized SMAs

It is well known that the melting temperature,  $T_m$  in low-dimensional materials can be changed by treating the interface [33–35]. For example, the phenomenon of premelting is commonly

observed in free-standing nanometer-sized metal particles, while superheating can be obtained when coated by (or embedded in) a high- $T_m$  materials. The main reason for the different melting behavior is the interface energy [34,36]. For nanosized SMAs, a similar strategy can be used to change structural phase transformations. Here  $\Delta\gamma$  is defined as the interface energy difference between product phase and parent phase, i.e.  $\Delta\gamma = \gamma_M - \gamma_P$ . If a transformation process can reduce the interface energy ( $\Delta\gamma < 0$ ), MT nucleation in the near-interface region will be energetically preferred compared to its bulk counterpart. By contrast,  $\Delta\gamma > 0$  indicates a suppressing effect on the MT nucleation in this region. Actually, this idea has been used to explain an inverse martensitic transformation in Zr nanowires [37].

We then derive the relation between transformation temperature and sample size thermodynamically. In analogy with surface melting, we identify the MT by equating the Gibbs free energy  $\mu_P$  and  $\mu_M$  of the parent and product phase in nanosized SMA, and the free energy is assumed to be a function of temperature  $T_0$  and pressure  $p_0$ :

$$\mu_P(p_0, T_0) = \mu_M(p_0, T_0) \quad (1)$$

This equation means that the free energies of a fully parent phase and martensite are equal at the transition temperature. The free energy can be expanded around its value at the critical point (i.e., transition temperature  $T_0^{\text{bulk}}$  or transition pressure  $p_0^{\text{bulk}}$ ), and we retain first-order terms only:

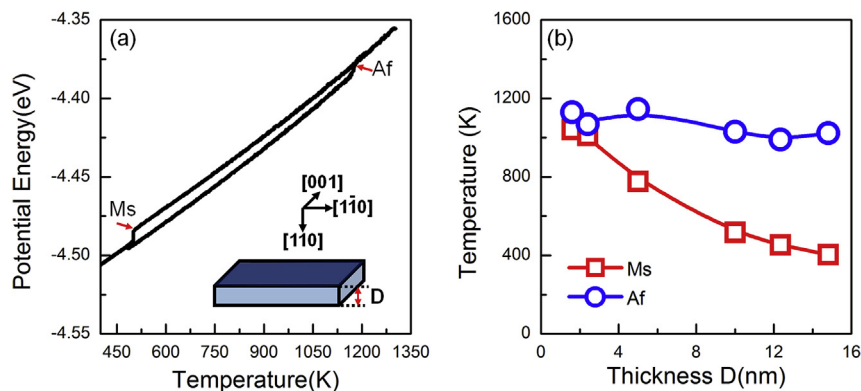
$$\mu(p_0, T_0) = \mu^{\text{bulk}}(p_0^{\text{bulk}}, T_0^{\text{bulk}}) + \frac{\partial\mu}{\partial T}(T_0 - T_0^{\text{bulk}}) + \frac{\partial\mu}{\partial p}(p_0 - p_0^{\text{bulk}}) \quad (2)$$

From the Gibbs–Duhem equation ( $-Vdp + SdT + Nd\mu = 0$ ) it follows that

$$\frac{\partial\mu}{\partial T} = -s, \quad \frac{\partial\mu}{\partial p} = \frac{1}{\rho} \quad (3)$$

where  $s = S/n$  is the entropy per atomic and  $\rho = n/V$  is the number density. Combined with Equations (1)–(3), and taking into account that  $\mu_P^{\text{bulk}}(p_0^{\text{bulk}}, T_0^{\text{bulk}}) = \mu_M^{\text{bulk}}(p_0^{\text{bulk}}, T_0^{\text{bulk}})$ , we obtain:

$$\begin{aligned} -s_P(T_0 - T_0^{\text{bulk}}) + \frac{1}{\rho_P}(p_P - p_0^{\text{bulk}}) \\ = -s_M(T_0 - T_0^{\text{bulk}}) + \frac{1}{\rho_M}(p_M - p_0^{\text{bulk}}) \end{aligned} \quad (4)$$



**Fig. 1.** The film thickness dependent martensitic transformation characteristic temperatures in free-standing (110)  $\text{Ni}_{63.5}\text{Al}_{37.5}$  monolayer. (a) Variation of the average potential energy of a  $\text{Ni}_{63.5}\text{Al}_{37.5}$  film with 10 nm in thickness during cooling and heating. The inset shows the crystallographic orientation of the (110)  $\text{Ni}_{63.5}\text{Al}_{37.5}$  monolayer simulated. (b) The transformation temperatures,  $M_s$  and  $A_f$  (arrows in a), as a function of the film thickness  $D$ .

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