



Full length article

# Taming martensitic transformation via concentration modulation at nanoscale



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## ARTICLE INFO

### Article history:

Received 10 February 2017

Received in revised form

16 March 2017

Accepted 17 March 2017

Available online 24 March 2017

### Keywords:

Concentration modulation

Martensitic transformation

Hysteresis

Pseudo-elasticity

Computer simulation

## ABSTRACT

Martensitic transformation (MT) is typically a strongly first-order transition with autocatalysis in nucleation followed by rapid growth. It usually takes place within a narrow temperature or stress range, making its utilization in a controllable manner difficult. We show by computer simulations how MTs can be tailored by concentration modulation at the nanoscale in the parent phase, which induces spatial variations of both the stability of martensite and the transformation strain and tunes the overall MT kinetics from a typical first-order transition into a high-order like continuous transition. Such a unique MT characteristic reduces or even eliminates the transformation hysteresis and produces quasi-linear elasticity with ultra-low apparent elastic modulus.

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## 1. Introduction

For an important class of smart materials, the shape memory alloys (SMAs), their functionalities (including shape memory effect and pseudo-elasticity) originate from martensitic transformations (MTs) [1,2]. MTs, being strongly first-order in nature [3], normally take place in an avalanche-like manner within a narrow temperature or stress range [4,5] and are accompanied by structural defects, large stress-strain or temperature-strain hysteresis and strongly nonlinear pseudo-elasticity, which leads to a variety of problems in applications [6,7]. For example, structural defects generate irrecoverable strain and cause functional fatigue and dimensional instability, which limits the service life of devices [7]. Even for the most widely used commercial SMA, NiTi, the irrecoverable strain may approach 10% after 100 thermal cycles under a 150 MPa bias load [8], and failure by fracture would occur after a few thousand cycles [9]. In addition, the efficiency of SMA actuators is often less

than 1% in practical applications due to large hysteresis, which is lower by several tens of times than that of piezo ceramic actuators and hydraulic actuators [6]. Moreover, precise position control of actuators is required in micro-electromechanical systems, e.g., robotics and active catheters, but the strongly nonlinear pseudo-elasticity of SMAs makes such control difficult [10–12].

Extensive studies have been carried out lately to tailor the stress-strain or temperature-strain responses and ameliorate degradation of SMAs. It has been shown that SMAs with high reversibility and low hysteresis can be developed by improving the geometrical compatibility between the parent and martensitic phases [13–17]. But the strict requirement on the transformation strain makes this approach applicable only to limited material systems (i.e. Ti–Ni–Cu–Pd and Zn–Au–Cu). Additionally, it has been shown theoretically that a giant non-hysteretic strain response could be achieved if the structural anisotropy of a low-symmetry phase vanishes [18], but experimental validation of this prediction has yet to come. Very recently, superelasticity with low hysteresis in a wide temperature range was found in Fe-, Co-, Cr-, Mn-doped TiNi system [19–21], Ni-rich TiNi alloys [22,23], Ni–Mn alloys [24] and AuCuAl alloys [25] under the assistance of strain glass transitions. Unfortunately, strain glass transitions are found so far only in ferroelastic systems having small transformation strains like

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the R phase in TiNi SMAs [26]. However, both experimental [20,23] and simulation [19,26] studies on strain glass transitions have demonstrated that the hysteresis of MTs can be tuned if the sharp first-order transition could be converted into a broadly smeared high-order like transition and that functional fatigue and nonlinear pseudo-elasticity can be effectively inhibited by reducing the transition hysteresis [16,18,19,27].

It is well documented that MT is sensitive to alloy composition [2,28–30]. In nitinol, for example, one atomic percent variation in Ni concentration could change the MT start temperature ( $M_s$ ) by ~100 K [30]. Similar phenomena are also found in other SMAs and GUM metals, including TiNb [31,32], TiMo [33], AuCuZn [16], and CuAl-based [1] alloys. In addition to  $M_s$ , alloy composition may also have a strong effect on the transformation strain [31,34,35]. This suggests that concentration modulation (CM) in the parent phase could be an effective way of altering the nature of MTs. For example, it has been reported that the superelasticity and thermal expansion of Ti2448 (Ti-24Nb-4Zr-8Sn-0.100 in wt.%) can be tuned by regulating the MT by CMs [36]. In Ti-Nb, there exist a large miscibility gap, with a spinodal range between ~10 and ~90 at.% of Nb [37]. The hysteresis and stress window for the MT in this system are found to be sensitive to alloy composition and solution heat treatment schedule [31]. Additionally, the spinodally decomposed Mn-Cu alloy is found to have a much higher  $M_s$  than its uniform concentration counterpart dose and the  $M_s$  shifts to higher temperatures with longer holding time during the spinodal decomposition [38,39]. As a matter of fact, CMs generated by spinodal decomposition are widely observed in SMAs, including TiNb [37,40], MnCu [38,39], TiV [41], FeMn [42] alloys, etc., with wavelengths ranging from several to several hundreds of nanometers [42]. Thus CMs generated via spinodal decomposition [43] in the parent phase could be utilized to alter the nature of MTs in SMAs. However, the detailed features of MTs in a compositionally modulated system remain largely unexplored.

In this study, we investigate by computer simulation how CMs at the nanoscale produced by spinodal decomposition in the parent phase affect the nature of MT in TiNb-based SMAs. We hypothesize that a spatial modulation in  $M_s$  accompanying the CM will make the MT highly heterogeneous and occur in a broad temperature range, while a transformation strain modulation will lead to different geometrical compatibility between the parent and martensitic phases and hence different local stress states. The simulation results and analyses suggest that introducing spatial modulation of concentration in the parent phase at the nanoscale is indeed able to convert the otherwise strongly first-order MT into an overall (or macroscopically) continuous transformation with slim hysteresis, quasi-linear pseudo-elasticity with large work output, and ultra-low apparent elastic modulus. Furthermore, strong fatigue resistance and Invar and Elinvar anomalies [36,44] could also be expected because of the continuous nature of the MT.

## 2. Phase field model

### 2.1. Symmetry breaking during MT in TiNb-based SMAs

A phase field model is formulated for the multifunctional  $\beta$  TiNb-based alloys. According to the Burgers lattice correspondence (LC) [45] for the  $\beta$  (BCC, point group  $m\bar{3}m$ ) to  $\alpha'$  martensite (orthorhombic, point group  $mmm$ ) transformation [46]

$$[001]_{\beta} \rightarrow [100]_{\alpha'}, [1\bar{1}0]_{\beta} \rightarrow [010]_{\alpha'}, [110]_{\beta} \rightarrow [001]_{\alpha'},$$

and the symmetry operations in the point groups that preserve such an LC, only 8 operations (out of the 48 symmetry operations in

$m\bar{3}m$ ) [47] are left after the transformation, leading to 6 (=48/8) crystallographic equivalent deformation modes (or correspondence variants) [48] characterized by 6 different transformation strain tensors. In fact, because an internal shuffle of  $\{110\}_{\beta}$  atomic planes is also involved during the transformation [49–51], which doubles the deformation variants, there are 12 deformation variants in total [52]. However, an internal shuffle dose not contribute to the transformation strain [3]. Thus, if we choose the three orthogonal axes of the cubic crystal of the parent phase as the reference coordinate system, as shown in Fig. 1(a), and follow the Burgers correspondence, the transformation matrices that map the parent phase lattice onto that of the martensitic variants by a uniform affine deformation read

$$\begin{aligned} \mathbf{U}_1 &= \begin{bmatrix} \zeta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{4} & \frac{\gamma-\alpha}{4} \\ 0 & \frac{\gamma-\alpha}{4} & \frac{\alpha+\gamma}{4} \end{bmatrix}, \mathbf{U}_2 = \begin{bmatrix} \zeta & 0 & 0 \\ 0 & \frac{\alpha+\gamma}{4} & \frac{\alpha-\gamma}{4} \\ 0 & \frac{\alpha-\gamma}{4} & \frac{\alpha+\gamma}{4} \end{bmatrix}, \\ \mathbf{U}_3 &= \begin{bmatrix} \frac{\alpha+\gamma}{4} & 0 & \frac{\gamma-\alpha}{4} \\ 0 & \zeta & 0 \\ \frac{\gamma-\alpha}{4} & 0 & \frac{\alpha+\gamma}{4} \end{bmatrix}, \mathbf{U}_4 = \begin{bmatrix} \frac{\alpha+\gamma}{4} & 0 & \frac{\alpha-\gamma}{4} \\ 0 & \zeta & 0 \\ \frac{\alpha-\gamma}{4} & 0 & \frac{\alpha+\gamma}{4} \end{bmatrix}, \\ \mathbf{U}_5 &= \begin{bmatrix} \frac{\alpha+\gamma}{4} & \frac{\gamma-\alpha}{4} & 0 \\ \frac{\gamma-\alpha}{4} & \frac{\alpha+\gamma}{4} & 0 \\ 0 & 0 & \zeta \end{bmatrix}, \mathbf{U}_6 = \begin{bmatrix} \frac{\alpha+\gamma}{4} & \frac{\alpha-\gamma}{4} & 0 \\ \frac{\alpha-\gamma}{4} & \frac{\alpha+\gamma}{4} & 0 \\ 0 & 0 & \zeta \end{bmatrix}. \end{aligned} \quad (1)$$

where  $\alpha = \sqrt{2}b/a_0$ ,  $\zeta = a/a_0$ ,  $\gamma = \sqrt{2}c/a_0$ , with  $a_0$ ,  $a$ ,  $b$  and  $c$  being the lattice parameters of the parent and martensitic phase, respectively, as shown in Fig. 1(a). The corresponding stress-free transformation strain (SFTS) of the  $p$ -th variant,  $\varepsilon_{ij}^0(p)$ , can be calculated directly from the transformation matrices given in Eq. (1) according to the following equation

$$\varepsilon_{ij}^0(p) = \frac{1}{2} (\mathbf{U}_p^T \mathbf{U}_p - \mathbf{I}), (p = 1 \sim 6), \quad (2)$$

where the superscript  $T$  indicates matrix transpose, and  $\mathbf{I}$  is the identity matrix.

Note that we are considering a compositionally non-uniform system in the current study and the lattice parameters of the parent and martensitic phases are functions of local concentration, which makes the SFTS in Eq. (2) a function of location as well. Both experimental measurements [31] and *ab initio* calculations [53] show that the concentration-dependence of lattice parameters of  $\beta$  and  $\alpha'$  phases in TiNb-based alloys can be approximated by linear functions (i.e., following the Vegard's law). Therefore in the simulations the variations of lattice parameters of  $\beta$  and  $\alpha'$  phases with concentration are obtained by fitting the data reported in the literature [31,34,46,53,54] to linear functions, i.e.,

$$a_0 = 3.296 + 1.3 \times c_{Nb} \times 10^{-4} \text{ \AA}, \quad (3a)$$

$$a = 2.894 + 1.2 \times c_{Nb} \times 10^{-2} \text{ \AA}, \quad (3b)$$

$$b = 5.167 - 1.7 \times c_{Nb} \times 10^{-2} \text{ \AA}, \quad (3c)$$

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