



# Microstructural analysis and molecular dynamics modeling of shape memory alloys



Chia-Wei Yang, Nien-Ti Tsou\*

Department of Materials Science and Engineering, National Chiao Tung University, Ta Hsueh Road, Hsinchu 300, Taiwan

## ARTICLE INFO

### Article history:

Received 17 November 2016  
Received in revised form 10 February 2017  
Accepted 12 February 2017

### Keywords:

Shape memory alloys  
Microstructure  
Molecular dynamics  
Crystal variant

## ABSTRACT

Molecular dynamics (MD) is an effective tool for studying the microstructures in shape memory alloys at the atomic level. However, microstructural analysis of the results generated by MD is typically done by examining lattice constants or monoclinic angles, and only a limited set of the crystal variants can be identified. In the current work, a numerical method that can identify the crystal variants and multiple phases is proposed. By observing the pattern of the components in the transformation matrix of the lattice in the crystal, the corresponding variant of the lattice can be determined. The method is then applied to study the martensitic transformation induced by temperature and ultrahigh shear strain, and the resulting microstructures are verified by literature. Moreover, the microstructural evolution and the volume fraction variation of the crystal variants under ultrahigh shear strain are examined. The observed multiple stages of phase transitions imply that the current method is able to identify the austenitic, orthorhombic, trigonal (*R* phase), monoclinic, and body-centered orthorhombic crystal systems simultaneously. The proposed method also reveals that the nanometer-sized *R* phase is a transition zone that maintains the compatibility between the two phases in the different crystal systems. The proposed method is rapid, accurate, and sufficiently versatile to be applicable to other crystal systems and related materials.

© 2017 Elsevier B.V. All rights reserved.

## 1. Introduction

Shape memory alloys (SMAs) are one of the most important types of metal alloys. They possess unique properties such as shape memory effect and superelasticity, thus enabling their wide use as actuators and stents, among other industrial applications. Their properties are governed by the well-known martensitic transformation and the corresponding microstructural evolution. For example, Ullakko et al. [1] reported that the large, reversible field-induced strain in magnetic SMAs is caused by the rearrangement of the microstructure. Liu [2] also found that the twin and detwinned microstructures play important roles in the level of shape recovery.

The microstructures in SMAs have been extensively studied by using theoretical modeling. For example, Knüpfer and Kružík [3] proved the existence of an energetic solution of the SMA microstructure in the rate-independent evolutionary model. Lei et al. [4] developed a two-scale phase field model to study the effect of the middle eigenvalue of martensite transformation strain on the stability of the austenite–martensite interfaces. Maletta

et al. [5] studied microstructural evolution due to indentation by using the finite element method. Pun and Mishin [6] utilized molecular dynamics (MD) simulation with an embedded-atom interatomic potential in order to study the effect of chemical composition and uniaxial mechanical stresses on the martensitic transformation in Ni-rich NiAl alloys.

Among these approaches, MD is an effective tool when used to investigate the properties and behavior of materials at the atomic level. It allows the prediction of the microstructure that a material forms on the basis of its interatomic potential and local strain state. This approach is particularly suitable for explaining macroscopic properties and for providing atomic-level insight into the solid–solid phase transition. The Finnis–Sinclair (FS) potential [7] is widely used in MD simulations to describe the behavior of Ni–Ti-based SMAs. Mutter and Nielaba [8] used this potential to visualize the microstructure and then examined the orientation of austenite–martensite interfaces in spherical Ni–Ti nanoparticles. Sushko et al. [9] studied the dependence of microstructural deformations on the type of the indenter. Tehrani et al. [10] modeled the point defects observed in the martensitic transformation. Zhong et al. [7] modified the FS potential and found the relationship between dislocation pinning and irreversible twinning. Mirzaeifar

\* Corresponding author.

E-mail address: [tsounienti@nctu.edu.tw](mailto:tsounienti@nctu.edu.tw) (N.-T. Tsou).

et al. [11] showed the unique formation of compound twins that dominate the nanostructure of Ni–Ti alloys subjected to loads.

The trajectories generated by MD simulation require post-processing analysis in order to obtain the properties of interest from the atomic positions stored as a function of time. In the present study, the properties of interest are: the strain, stress and, particularly, the phase/variant in each lattice. In the literature, phase formation is typically identified by the transformed lattice constants and monoclinic angle ( $\gamma$ ), e.g.,  $\gamma = 90^\circ$  for the austenitic phase and  $\gamma \approx 98^\circ$  for the monoclinic phase [7]. The martensite variants are typically distinguished by the order parameter, which is also defined by the lattice constants [11]; however, only a limited set of the variants can be identified. Wu et al. [12] identified martensite variants in their MD model by matching the transformation matrix with the target matrix obtained separately by MD simulations of single variants. The calculation is tedious, however, and the target matrices are applicable only to particular cases because the lattice constants vary with the temperature [13]. A numerical method that can reveal details of the SMA microstructure, such as the volume fraction of the martensite variants present in the crystal and the occurrence of an intermediate phase during martensitic transformation, is therefore still desirable.

The development of such a model is the motivation behind the current study. Herein we develop a post-processing algorithm that can identify the crystal system and corresponding variants of the lattice in the atomistic model. This is achieved by tracking the position of the atoms at the corners of each lattice in the MD simulation and by checking the similarity of the determined transformation matrix to the ideal one for each variant in all possible crystal systems in the SMAs [13]. The crystal variant of that lattice can then be identified as the variant with the most similar ideal transformation matrix. In the present work, the method is applied to several cases of the MD simulation for Ni–Ti SMAs in which the FS interatomic potential [7] is used. Results generated by other researchers [11] and the well-known compatibility equation [13] confirm the results. Moreover, the microstructural evolution of the Ni–Ti SMA due to ultrahigh strain is simulated. We capture the feature of a mixture of multiple martensite phases in the SMA, including the intermediate *R* phase and the base-centered orthorhombic (*BCO*) phase. The volume fraction of the crystal variants and the corresponding stress–strain curve are also evaluated. The proposed post-processing method enables the efficient exploration of the phase transitions and microstructures in the SMAs. It is expected to be applicable to other related materials with similar phase/variant transition, such as ferroelectric materials.

## 2. Theory and methodology

### 2.1. Algorithm for identifying the crystal variants

Many possible crystal systems and martensite variants may exist during the phase transition of Ni–Ti SMAs. Possible crystal systems reported in literature are austenite (*A*), trigonal (*R*), orthorhombic (*O*), monoclinic (*M*), and *BCO* phases consisting of 1, 4, 6, 12, and 12 crystal variants, respectively. Each of the variants has a distinct transformation matrix,  $\mathbf{U}$ , which describes the distortion of the lattice from the reference state, with the *A* phase possessing a unity transformation matrix. With the monoclinic crystal system used as an example, the 12 ideal transformation matrices are listed in Table 1, where  $\alpha$ ,  $\varepsilon$ ,  $\gamma$ , and  $\delta$  are material properties, e.g.  $\alpha = 1.0243$ ,  $\gamma = 0.9563$ ,  $\delta = 0.058$ , and  $\varepsilon = -0.0427$  for Ni-49.75 at.%Ti [13]. Patterns for the components of these ideal transformation matrices can be observed. These ideal matrices are symmetric; therefore, we consider here the components in the upper

**Table 1**  
Transformation matrices for the cubic-to-monoclinic transition.

$\mathbf{U}_1 = \begin{bmatrix} \gamma & \varepsilon & \varepsilon \\ \varepsilon & \alpha & \delta \\ \varepsilon & \delta & \alpha \end{bmatrix}$ ,	$\mathbf{U}_5 = \begin{bmatrix} \alpha & \varepsilon & \delta \\ \varepsilon & \gamma & \varepsilon \\ \delta & \varepsilon & \alpha \end{bmatrix}$ ,	$\mathbf{U}_9 = \begin{bmatrix} \alpha & \delta & \varepsilon \\ \delta & \alpha & \varepsilon \\ \varepsilon & \varepsilon & \gamma \end{bmatrix}$ ,
$\mathbf{U}_2 = \begin{bmatrix} \gamma & -\varepsilon & -\varepsilon \\ -\varepsilon & \alpha & \delta \\ -\varepsilon & \delta & \alpha \end{bmatrix}$ ,	$\mathbf{U}_6 = \begin{bmatrix} \alpha & -\varepsilon & \delta \\ -\varepsilon & \gamma & -\varepsilon \\ \delta & -\varepsilon & \alpha \end{bmatrix}$ ,	$\mathbf{U}_{10} = \begin{bmatrix} \alpha & \delta & -\varepsilon \\ \delta & \alpha & -\varepsilon \\ -\varepsilon & -\varepsilon & \gamma \end{bmatrix}$ ,
$\mathbf{U}_3 = \begin{bmatrix} \gamma & -\varepsilon & \varepsilon \\ -\varepsilon & \alpha & -\delta \\ \varepsilon & -\delta & \alpha \end{bmatrix}$ ,	$\mathbf{U}_7 = \begin{bmatrix} \alpha & -\varepsilon & -\delta \\ -\varepsilon & \gamma & \varepsilon \\ -\delta & \varepsilon & \alpha \end{bmatrix}$ ,	$\mathbf{U}_{11} = \begin{bmatrix} \alpha & -\delta & \varepsilon \\ -\delta & \alpha & -\varepsilon \\ \varepsilon & -\varepsilon & \gamma \end{bmatrix}$ ,
$\mathbf{U}_4 = \begin{bmatrix} \gamma & \varepsilon & -\varepsilon \\ -\varepsilon & \alpha & -\delta \\ -\varepsilon & -\delta & \alpha \end{bmatrix}$ ,	$\mathbf{U}_8 = \begin{bmatrix} \alpha & \varepsilon & -\delta \\ \varepsilon & \gamma & -\varepsilon \\ -\delta & -\varepsilon & \alpha \end{bmatrix}$ ,	$\mathbf{U}_{12} = \begin{bmatrix} \alpha & -\delta & -\varepsilon \\ -\delta & \alpha & \varepsilon \\ -\varepsilon & \varepsilon & \gamma \end{bmatrix}$ .

**Table 2**  
The 15 conditions that can distinguish all variants in the *A*, *R*, *O*, and *M/BCO* phases in Ni–Ti SMAs.

A. $ u_{12}  -  u_{13}  < 2\emptyset$	J. $u_{12} > \emptyset$
B. $ u_{22}  -  u_{33}  < 2\emptyset$	K. $u_{13} > \emptyset$
C. $ u_{12}  -  u_{23}  < 2\emptyset$	L. $u_{23} > \emptyset$
D. $ u_{11}  -  u_{33}  < 2\emptyset$	M. $u_{12} < -\emptyset$
E. $ u_{13}  -  u_{23}  < 2\emptyset$	N. $u_{13} < -\emptyset$
F. $ u_{11}  -  u_{22}  < 2\emptyset$	O. $u_{23} < -\emptyset$
G. $ u_{12}  < \emptyset$	
H. $ u_{13}  < \emptyset$	
I. $ u_{23}  < \emptyset$	

triangular part only. For example, two of the diagonal components are identical to the  $\alpha$  value; two of the off-diagonal components have an identical absolute value of  $\varepsilon$ . These coefficients are located differently, and both  $\varepsilon$  and  $\delta$  are present with or without the negative sign, giving rise to the 12 monoclinic crystal variants. Similar patterns can also be found in the transformation matrices for the *O* and *R* crystal systems, as listed in Tables A1 and A2. These patterns allow distinction among the variants and crystal system.

On the basis of the inspection, we conclude that there are 15 conditions that can distinguish variants among the *A*, *R*, *O*, and *M/BCO* phases, as shown in Table 2. Here,  $u_{ij}$  is the component ( $i$ ,  $j$ ) of  $\mathbf{U}$ . First, we check if any pair of components in the diagonal and off-diagonal parts of the matrix have identical absolute values, giving six conditions (listed as A–F in Table 2).  $\emptyset$  is the tolerance that allows the small shift of the component due to thermal vibration in the MD simulation. Second, we check for any zero components, i.e., whether the absolute value of the component is less than the tolerance for the off-diagonal part, giving rise to the conditions G, H, and I. These conditions are set to distinguish the *O* and *A* phases from the other systems. Next, the signs of the components in the off-diagonal part producing the six conditions J–O are examined.

Table 3 is the characteristic table in which the matching conditions for each variant are listed. The transformation matrix of the *A* phase is an identity matrix and thus satisfies conditions A–I. Two independent nonzero components in the diagonal and off-diagonal are included in the transformation matrix of the *R* phase parts to satisfy conditions A–F. The *R* phase variants can then be further identified from the placement of the negative sign. A typical transformation matrix of the *O* phase has three independent material coefficients and two zero components in the off-diagonal part. This requires five conditions to distinguish all six of the orthorhombic variants. The transformation matrix of the *M* phase includes four independent material coefficients, and all of its components are nonzero. It also requires five conditions to allow identification of the 12 variants. The characteristic table can be extended on the basis of the patterns of the transformation matrix of any other phase such as the tetragonal crystal system.

Download English Version:

<https://daneshyari.com/en/article/5453245>

Download Persian Version:

<https://daneshyari.com/article/5453245>

[Daneshyari.com](https://daneshyari.com)