



# Unique properties associated with normal martensitic transition and strain glass transition – A simulation study

Dong Wang<sup>a,b,\*</sup>, Yan Ni<sup>a</sup>, Jinghui Gao<sup>a</sup>, Zhen Zhang<sup>a</sup>, Xiaobing Ren<sup>a,c</sup>, Yunzhi Wang<sup>a,d</sup>

<sup>a</sup> Center for Computational Study of Microstructure Evolution in Materials, Multi-Disciplinary Materials Research Center, Frontier Institute of Science and Technology, State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, China

<sup>b</sup> State Key Laboratory for Strength and Vibration of Mechanical Structures, Xi'an Jiaotong University, Xi'an 710049, China

<sup>c</sup> Ferroic Physics Group, National Institute for Materials Science, Tsukuba 305-0047, Ibaraki, Japan

<sup>d</sup> Department of Materials Science and Engineering, The Ohio State University, 2041 College Road, Columbus, OH 43210, USA

## ARTICLE INFO

### Article history:

Received 31 October 2011

Received in revised form 5 January 2012

Accepted 1 March 2012

Available online 7 March 2012

### Keywords:

Point defect

Phase transformation

Nanodomains

Ferroelastic system

Phase field

## ABSTRACT

The transition behavior and unique properties associated with normal martensitic transition and strain glass transition are investigated by computer simulations using the phase field method. The simulations are based on a physical model that assumes that point defects alter the thermodynamic stability of martensite and create local lattice distortion. The simulation results show that strain glass transition exhibits different properties from those found in normal martensitic transformations. These unique properties include diffuse scattering pattern, “smear” elastic modulus peak, disappearance of heat flow peak and non-ergodicity. These simulation predictions agree well with the experimental observations.

© 2012 Elsevier B.V. All rights reserved.

## 1. Introduction

A normal ferroelastic is characterized by a transformation from austenite – a paraelastic state with disordered dynamic strain domains (i.e., a strain liquid) to martensite – a long range ordered strain domains as in a poly twined microstructure (i.e., a strain crystal) upon cooling [1,2]. The martensitic transformation shows typical first order transition behavior and plays an important role in advanced technological applications such as in shape memory alloys. Recently, a strain glass transition has been discovered in  $Ti_{50-x}Ni_{50+x}$  ferroelastic system when  $x > 1.0$  [3]. This strain glass transition is parallel to the well studied cluster-spin glass [4,5] in ferromagnetic systems and ferroelectric relaxor [6–8] in ferroelectric systems. A strain glass is neither a strain liquid nor a strain crystal, but a frozen disordered strain state with short range order. On one hand it is characterized by unique properties not found in normal ferroelastics, including “smear” elastic modulus peak with frequency dispersion, disappearance of heat flow peak, and small thermal hysteresis, while on the other hand, it exhibits

similar features as the martensite such as non-ergodicity indicated by ZFC/FC experiments [9–13], shape memory effect and superelasticity [9,10]. In addition, strain glass is different from the precursory tweed [14–16], which should be a kind of partially frozen strain states [13,17]. The unique frozen local strain order and special properties make strain glass indispensable for possible technology applications.

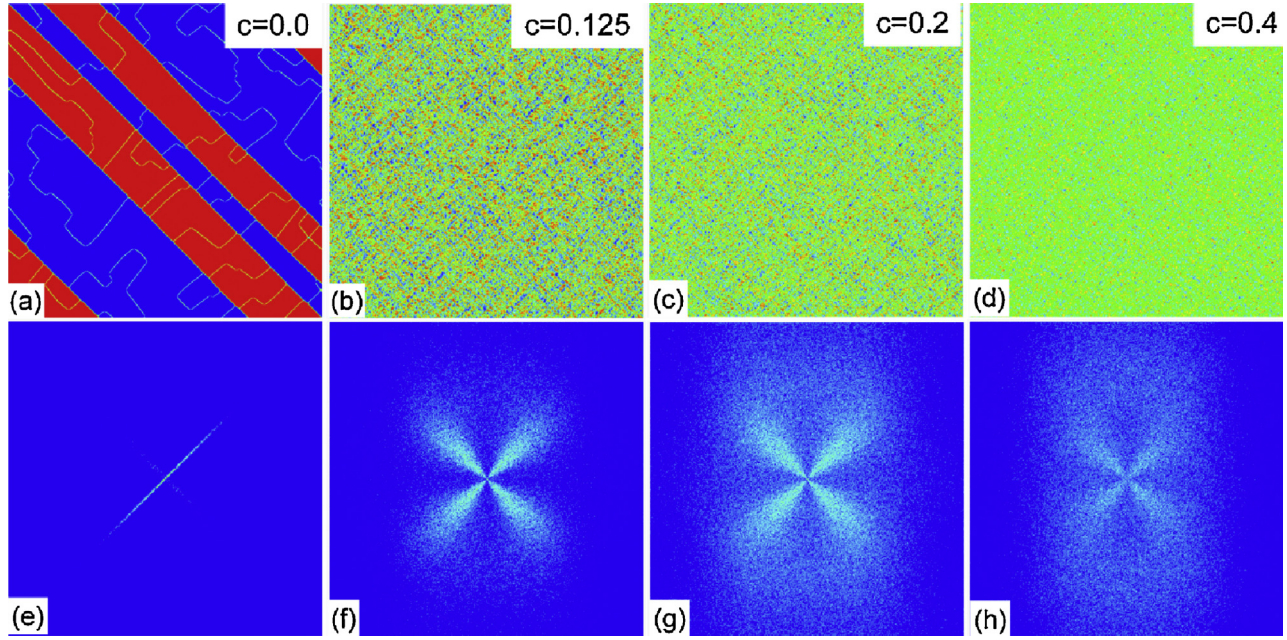
To understand the relationship among different strain states in doped ferroelastic systems, a phase field model based on Landau theory of phase transition has been developed [17]. In this model, point defects are assumed to alter the thermodynamic stability of martensite (i.e., global transition temperature effect GTTE) and create local lattice distortion (i.e., local field effect LFE). Computer simulations based on the model have reproduced the strain glass transition and described all the strain states. In the present paper, the same model [17] is used to study the transition behavior and unique properties of a strain glass system through phase field simulations. The simulations reproduced all the signature properties of a strain glass reported in recent experiments [9–13].

## 2. Model

The simulation is carried out for the improper square → rectangle (2D) MT in a single crystal constrained systems [18,19]. The order parameters of ‘rectangular’ martensitic

\* Corresponding author at: Center for Computational Study of Microstructure Evolution in Materials, Multi-Disciplinary Materials Research Center, Frontier Institute of Science and Technology, State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, China.

E-mail address: [wangdong1223@gmail.com](mailto:wangdong1223@gmail.com) (D. Wang).



**Fig. 1.** Microstructures of normal martensite at  $c=0.0$  and strain glass at  $c=0.125$ ,  $c=0.2$ , and  $c=0.4$ . (e–h) Describe the corresponding diffraction patterns. (a and e)  $c=0.0$ ; (b and f)  $c=0.125$ ; (c and g)  $c=0.2$ ; (d and h)  $c=0.4$ .

phase are described by two field variables:  $\eta(\mathbf{r})_1$ , and  $\eta(\mathbf{r})_2$  ( $\mathbf{r}$  is the coordinate vector). The stress-free transition strain  $\varepsilon_{ij}^0(\mathbf{r})$  at point  $\mathbf{r}$  as a function of the order parameters ( $\eta(\mathbf{r})_1$ , and  $\eta(\mathbf{r})_2$ ) [18,19]:

$$\varepsilon_{ij}^0(\mathbf{r}) = \varepsilon_{ij}^{00}(1)\eta(r)_1^2 + \varepsilon_{ij}^{00}(2)\eta(r)_2^2, \quad \text{where} \quad \varepsilon_{ij}^{00}(1) = \varepsilon_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

and  $\varepsilon_{ij}^{00}(2) = \varepsilon_0 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$  are the constant tensors and  $\varepsilon_0$  is the value of the transformation shear. The driving force of the square  $\rightarrow$  rectangle transformation is minimized by two sets of the long range order parameters mentioned above:  $(\eta_1, \eta_2) = (\eta_0, 0)$  and  $(\eta_1, \eta_2) = (0, \eta_0)$ , where  $\eta_0$  is the equilibrium value of the long range order parameter. The chemical free energy can be described:

$$F_{ch} = \int \left[ \frac{1}{2} \beta (\nabla \eta_1)^2 + \frac{1}{2} \beta (\nabla \eta_2)^2 + f(\eta_1, \eta_2) \right] d^2r, \quad (1)$$

$$f(\eta_1, \eta_2) = \frac{1}{2} A_1 (\eta(r)_1^2 + \eta(r)_2^2) - \frac{1}{4} A_2 (\eta(r)_1^4 + \eta(r)_2^4) + \frac{1}{4} A_3 (\eta(r)_1^2 + \eta(r)_2^2)^2 + \frac{1}{6} A_4 (\eta(r)_1^2 + \eta(r)_2^2)^3, \quad (2)$$

The global transition temperature effect caused by point defect has been described in the Landau term through changing the  $A_1$  value [18]:  $A_1 = A_1^0 + b \cdot c = A_1^{00} \cdot (T - T^0) + b \cdot c$ , where  $c$  is the concentration,  $b$  describes the defect strength,  $T^0$  is the critical transition temperature. The local field effect of point defects which is time independent and position dependent can be described through local strain  $\varepsilon_{loc\ ij}^0(\mathbf{r})$  at position  $\mathbf{r}$ :  $\varepsilon_{loc\ ij}^0(\mathbf{r}) = \varepsilon_{ij}^{00}(1)\eta(r)_{loc(1)} + \varepsilon_{ij}^{00}(2)\eta(r)_{loc(2)}$ ,  $\eta(r)_{loc(1)}$  and  $\eta(r)_{loc(2)}$  are the order parameters to describe local field [17]. According to the theory of local field effect in ferroelectric systems [20] and the understanding of strain glass transition [17], in present work, the local field effects have been described through adding odd term in Landau phenomenological free energy term [17].

$$f_L(\eta_1, \eta_2) = f(\eta_1, \eta_2) + \left[ \begin{array}{l} -\eta_{loc(1)} \left[ A_1(T_0)\eta(r)_1 - \frac{1}{3}(A_2 - A_3)\eta(r)_1^3 + A_3\eta(r)_2^2\eta(r)_1 + \frac{1}{5}A_4\eta(r)_1^5 + A_4\eta(r)_2^4\eta(r)_1 + \frac{2}{3}A_4\eta(r)_2^2\eta(r)_1^3 \right] \\ -\eta_{loc(2)} \left[ A_1(T_0)\eta(r)_2 - \frac{1}{3}(A_2 - A_3)\eta(r)_2^3 + A_3\eta(r)_1^2\eta(r)_2 + \frac{1}{5}A_4\eta(r)_2^5 + A_4\eta(r)_1^4\eta(r)_2 + \frac{2}{3}A_4\eta(r)_1^2\eta(r)_2^3 \right] \end{array} \right] \quad (3)$$

The first term in Eq. (3) depicts the normal Landau polynomial term (2) and the second and third terms describe the local field relevant odd term caused by local field effect [12,20].

The contribution of the transformation-induced coherency strain to the free energy is given by Khachatryan [18,21]. The stochastic time-dependent kinetic equation has been used to describe the temporal evolution.  $\eta_p(\mathbf{r}, t + \Delta t) = \eta_p(\mathbf{r}, t) + ((d\eta_p(\mathbf{r}, t))/dt)\Delta t$ , where  $(d\eta_p(\mathbf{r}, t))/dt = -M((\delta F)/(\delta \eta_p(\mathbf{r}, t))) + \xi_p(\mathbf{r}, t)$ ,  $p=1, 2$ . Kinetic equation was solved numerically using the Euler algorithm and a computational cell consisting of  $256 \times 256$  grid sites with periodical boundary conditions. To speed up the beginning of the kinetics process, we used large fluctuations  $\xi_p(\mathbf{r}, t)$ , which were produced by a random number generator.

The length scale in our simulation has been scaled in this simulation. The real interfacial energy  $\gamma$  for coherent face is  $\sim 0.05$  J/m<sup>2</sup> [22]. The chemical free energy  $\Delta F$  for martensitic transition system is about  $-1.85 \times 10^6$  J/m<sup>3</sup> ( $\sim 30$  J/mol) [23]. According to our simulation parameter, the length scale can be calculated according to the formula:  $\Delta F/\Delta F^* = \gamma/\gamma^*l_0$ .  $dx^* = dx/l_0$ , and we got  $dx^* \sim 0.94$  nm, which means the length of one grid in our simulation represent 0.94 nm in real materials.

### 3. Results and discussion

The microstructures at 250K obtained at different defect concentrations ( $c=0.0$ ,  $c=0.125$ ,  $c=0.2$ ,  $c=0.4$ ) are shown in Fig. 1(a)–(d). Fig. 1(e)–(h) shows the related diffuse scattering patterns obtained from the Fourier transform of  $|\eta_i(\mathbf{x})|^2$  at different defect concentrations. In the case of  $c=0.0$ , the system shows typical martensitic poly twined microstructures (see Fig. 1(a)) with strong long-range spatial correlations (as indicated by the diffraction pattern in Fig. 1(e)). When the defect concentration exceeds a critical value [17],  $c \sim 0.1$ , the nano-sized martensitic domains become randomly distributed in space and no longer transform

Download English Version:

<https://daneshyari.com/en/article/1613767>

Download Persian Version:

<https://daneshyari.com/article/1613767>

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