Phase-field simulations of thermomechanical behavior in MnNi shape memory alloys using finite element method

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Introduction: In 2D space, the square-to-rectangle transformation in Mn-Ni alloys was simulated, including the thermally induced transformation, the pseudoelastic behaviors during tensile and bending tests, the shape memory effects with free and constraint recoveries, and the strain-temperature relationship under constant stress. The simulation results of microstructure evolution and thermomechanical response were obtained and discussed.

Model and method:

Order parameter (η) is used to describe the microstructure field, and the temporal evolution of η is governed by the TDGL equation:

$$\frac{\partial \eta}{\partial t} = -L\frac{\delta G}{\delta \eta}$$

where L is the kinetic parameter. G is the total free energy of the system, which can be defined as the summation of the chemical free energy (G_{ch}), the gradient energy (G_{gr}), and the elastic strain energy (G_{el}):

$$G = G_{ch} + G_{gr} + G_{el}$$

$$G_{ch} = \int_V \left[\frac{A}{2}\eta^2 - \frac{B}{4}\eta^4 + \frac{C}{6}\eta^6\right]dV$$

$$G_{gr} = \int_V \frac{\beta}{2}(\nabla\eta)^2 dV \qquad G_{el} = \int_V \frac{1}{2}C_{ijkl}\varepsilon_{ij}^{el}\varepsilon_{kl}^{el}dV$$

$$\frac{\partial \eta}{\partial t} = -L\left(-\beta\nabla^2\eta + A\eta - B\eta^3 + C\eta^5 + \frac{\delta G_{el}}{\delta \eta}\right)$$

$$\frac{\delta G_{el}}{\delta \eta} = -\frac{1}{2}C_{ijkl}\left\{\varepsilon_{kl}^{00}\left[\frac{1}{2}(u_{i,j}+u_{j,i}) - \varepsilon_{ij}^{00}\eta\right] + \varepsilon_{ij}^{00}\left[\frac{1}{2}(u_{k,l}+u_{l,k}) - \varepsilon_{kl}^{00}\eta\right]\right\}$$

Results: 1. Thermally induced transformation

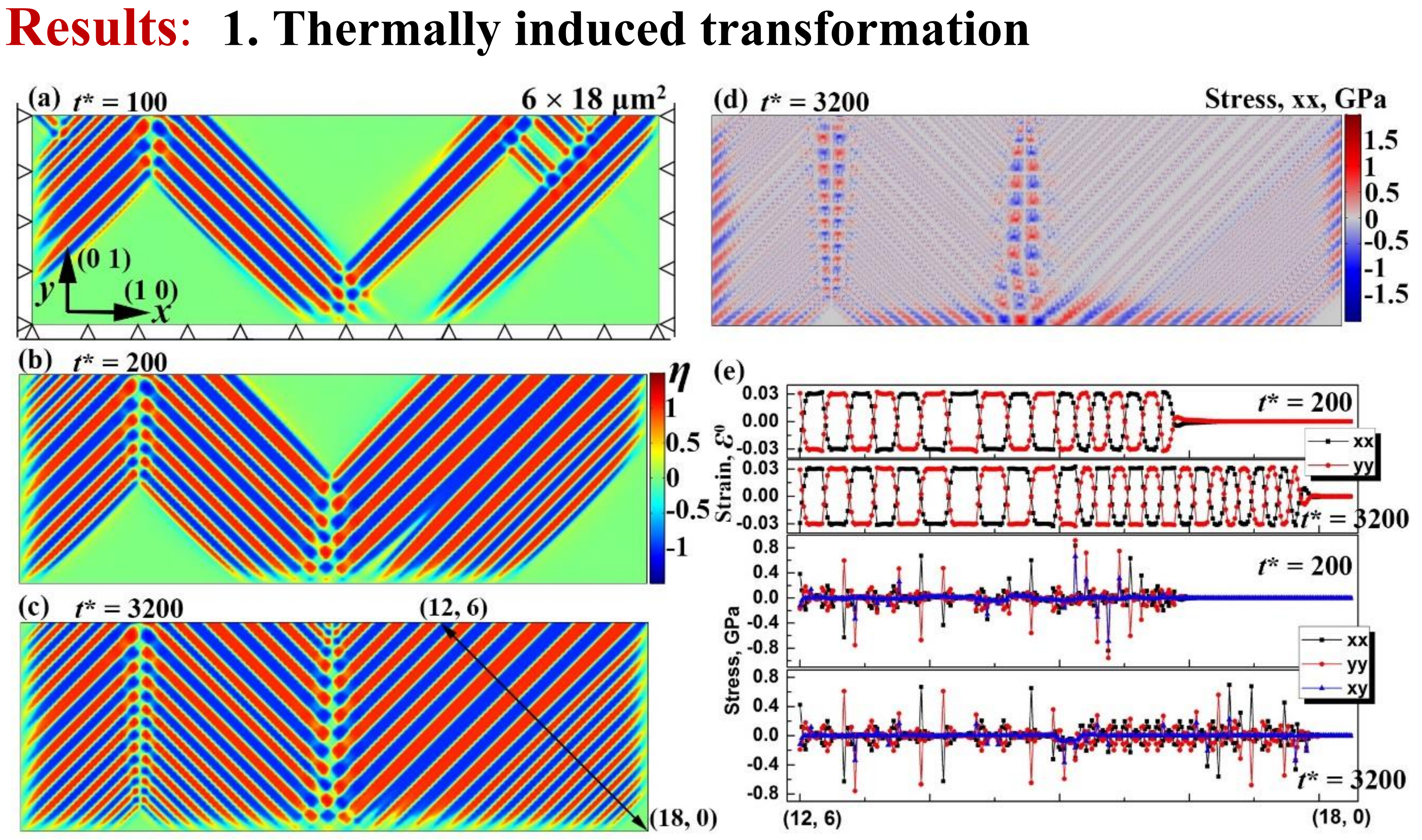

Fig. 1. Microstructure evolution during the thermally induced transformation at 432 K ((a), (b) and (c)), internal stress field retained in the material (d), and distribution of transformation strain and elastic stress along a [1 1̄] line (e).

Conclusions:

[1]FCT artensitic domains are observed during pseudoelastic bending.
[2]The coupling strength of SMA pipe coupling is enhanced
[3]Large shape change of SMAs is realized by the transition.

Results: 2. Pseudoelasticity

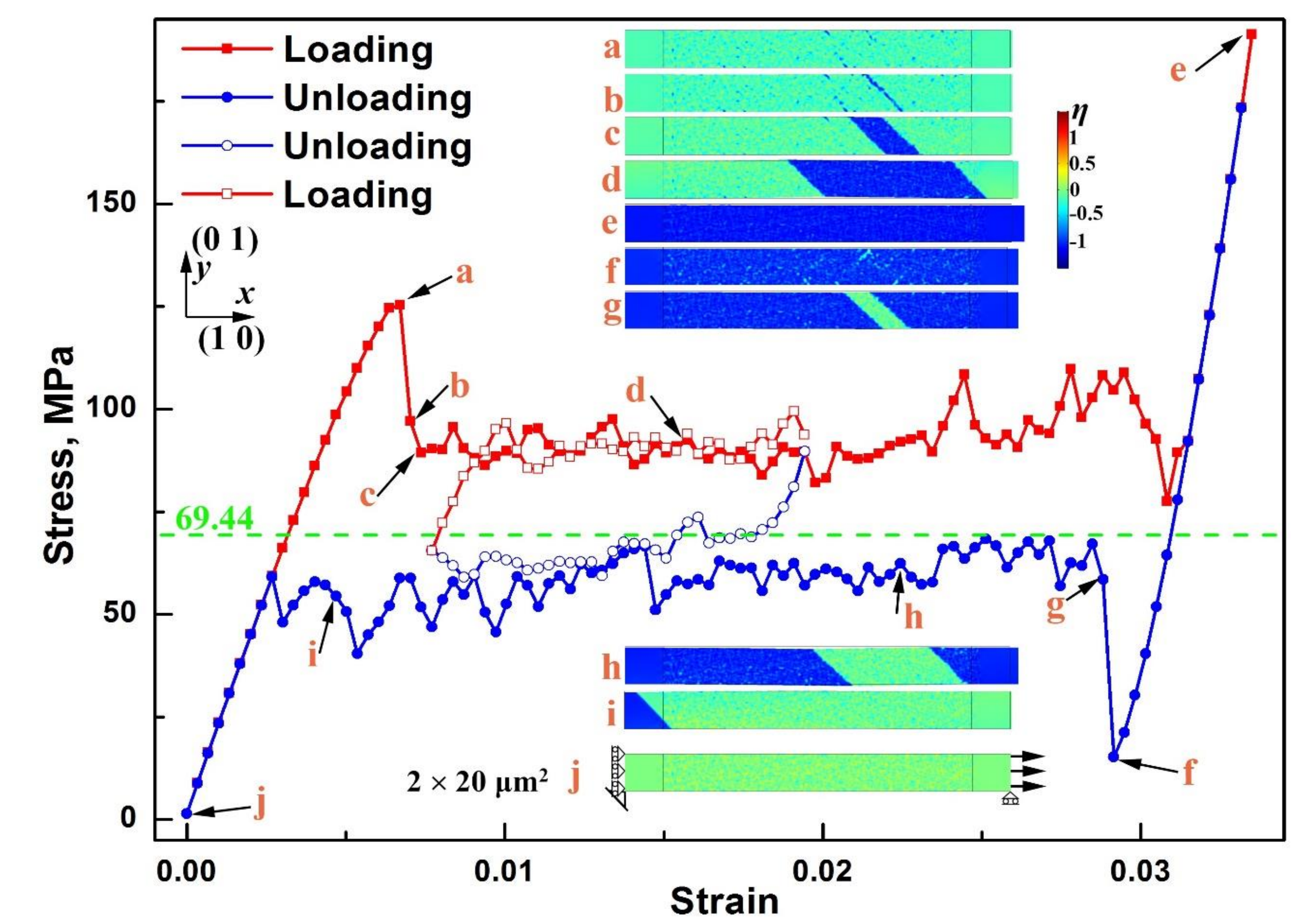

Fig. 2. Tensile stress-strain curve and associated microstructure evolution under displacement-controlled loading and unloading at 484 K (nominal strain rate of 1.3 □ 10-6 /s). A strain unloading and subsequent loading between 0.019 and 0.008 is shown with hollow symbols.

Results: 3. Shape memory effect

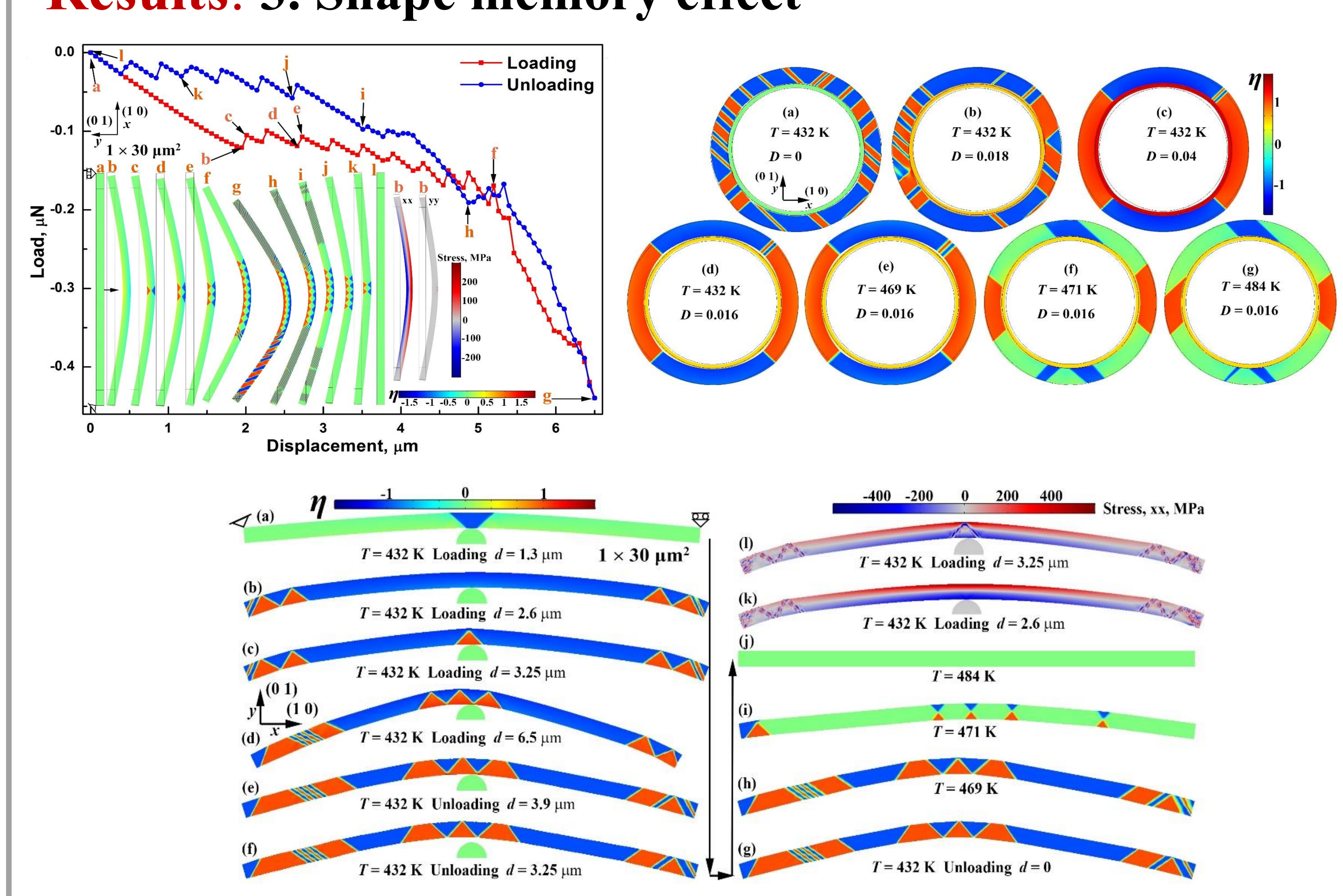

Fig. 3 SME under different shapes in the materials

Results: 4. Strain vs. temperature under constant load

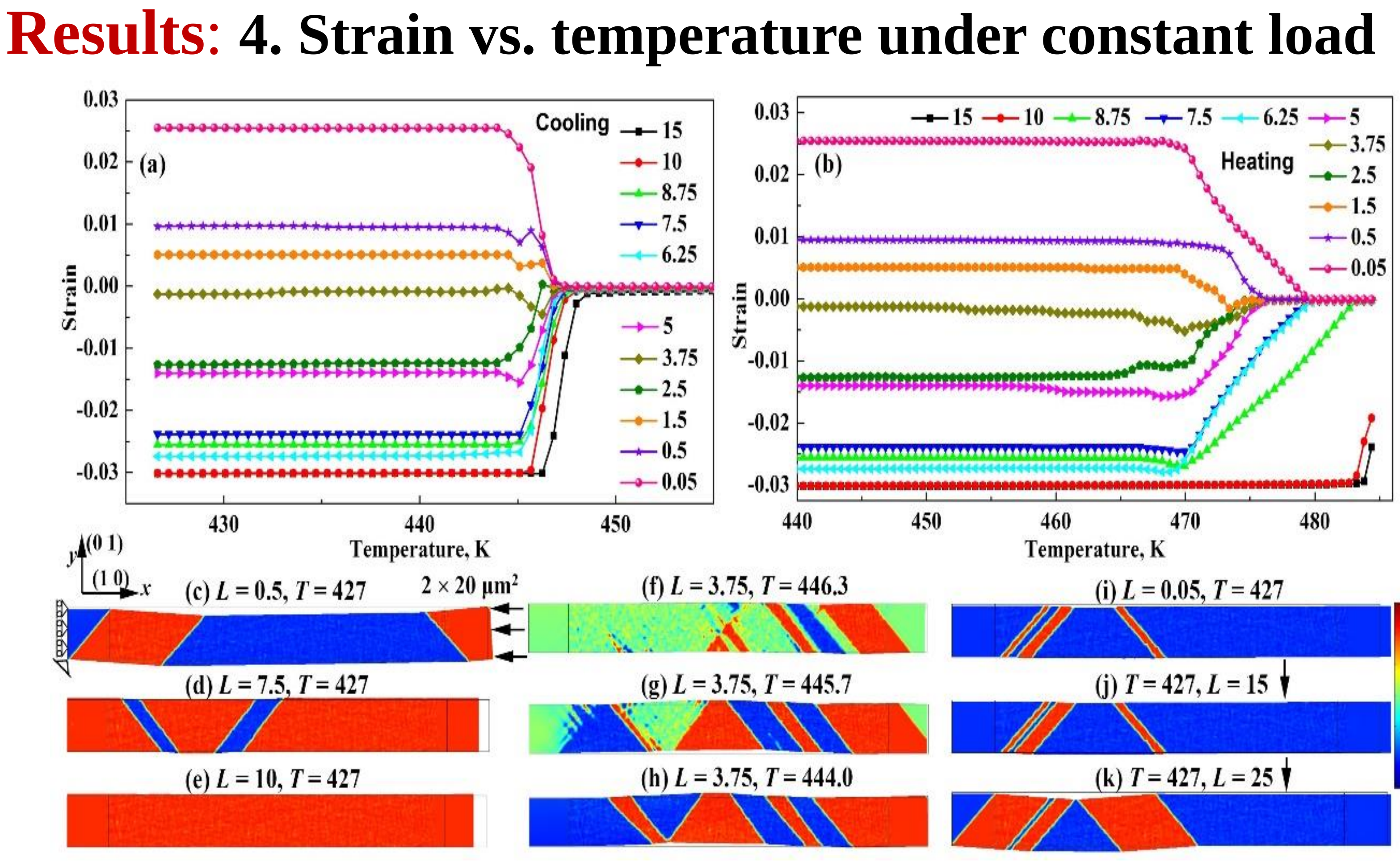

Fig. 9. The strain-temperature curves during cooling, subsequent heating and under various constant compressive stresses

References:

[1]Y. Wang, A. Khachaturyan, Three-dimensional field model and computer modeling of martensitic transformations, Acta Mater. 45 (1997) 759-773.
[2]COMSOL Multiphysics Users' Guide. Available from: http://www.comsol.com/.

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