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Dynamical phase-field modeling of one-dimensional ferroelastics under temperature and strain cycling

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ABSTRACT

A one-dimensional phase field model, based on a Landau-type free energy, is adopted to study the solid-solid phase transformation in ferroelastic materials, such as barium titanate, to model its negative-stiffness effects when undergoing phase transitions. Coupling between the order parameter, which describes spontaneous strain, and elastic strain is incorporated, as well as the domain wall strength, to model the mechanical responses of the material during transition under simultaneous thermal and mechanical loading. It is found that, with an initial random distribution of the order parameter, the several ferroelastic domains can be formed when constant temperature is less than the critical temperature Tc, and its evolution is monitored. Under the combined thermal and mechanical sinusoidal loading, the system exhibits anomalous effective stress-strain responses in the transient period. Smaller temperature rates prolong the anomalous behavior. When reaching equilibrium, the anomaly disappears.

1. INTRODUCTION

Ferroelastic materials exhibit hysteresis in the stress-strain curves (Salje 1990), which are analogously resembling to ferroelectric materials showing hysteresis in electric field vs. electric displacement curves and ferromagnetic materials showing hysteresis in magnetic field vs. induction field curves. Recent experiments have shown that composite materials containing ferroelastic inclusions may exhibit extreme effective properties, in terms of unbounded modulus and damping (Lakes et al. 2001) due to negative stiffness arises from the solid-solid phase transition. However, the direct use of negative values in elastic constants, even though it is legitimate, needs further justifications. In this study, we attempt to bridge the gaps in analyzing negative-stiffness composites by using the phase field modeling.

2. MATHEMATICAL MODEL

[1)] Associate Professor

The one-dimensional Helmholtz free energy density W(ε, p, T), a function of strain, polarization (i.e. order parameter) and temperature, also known as the Landau-Devonshire energy density (Zhang and Bhattacharya 2005), of the material that exhibits both ferroelectric and ferroelastic behavior, that is distinguished from the 'pure' ferroelastic material in which spontaneous polarization is not invoked in the transition.

$$W(e,p,T)=\frac{a_4}{6}p^6+\frac{a_2}{4}p^4+\frac{a(T-T_c)}{2}p^2+\frac{c_1}{2}e^2-\frac{b_1}{2}ep^2+\frac{k}{2}\left|\nabla p\right|^2 \quad (1)$$

The normalized Helmholtz free energy, as defined in Eq. (1), is calculated against prescribed spontaneous strain at end boundaries, as shown in Fig. 1, under the static assumption. It can be seen than the Helmholtz free energy of the system changes from a single well ($T > T_c$) to double well ($T < T_c$). As for time-evolution of the polarization domains, when under constant temperature loading $T < T_c$, stabilized domains can be formed; when $T > T_c$, polarization would become zero everywhere rapidly. In addition, to obtain stabilized domains, the parameter κ, that controls domain wall strength, must remain small.

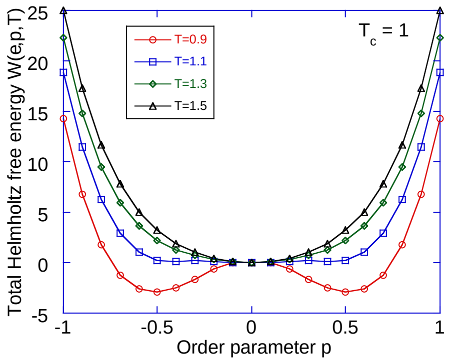

Fig. 1 Energy landscape of the 1D model with respect to spontaneous strain p

2. RESULTS AND DISCUSSION

Phase transformation kinetics was studied in terms of monitoring the time-evolution of field variables, and stability was tested by long-time calculations, as shown in Fig. 2. It was found that even though initial polarization distributions contain sharp gradients, such as random distribution, time-evolution according to the phase field model may smooth out the distribution. When equilibrium is reached, several domains can be stably formed, as shown in Fig. 2 (d).

Fig. 3 shows the results of combined thermal cycling and low-frequency sinusoidal straining. It can be seen that smaller temperature rates prolong the phase transition effects, giving rise to strain softening phenomenon in the short-time behavior. At longer time, no phase transition effects are detected, and the system follows the mechanical sinusoidal driving force with zero polarization. In our studies here, no negative stiffness values are directly assigned in our calculations, but the dynamical phase-field model reveals physical phenomena that resemble negative-stiffness composite systems, which is a direct consequence of changing of energy landscape during the ferroelastic phase transformation.

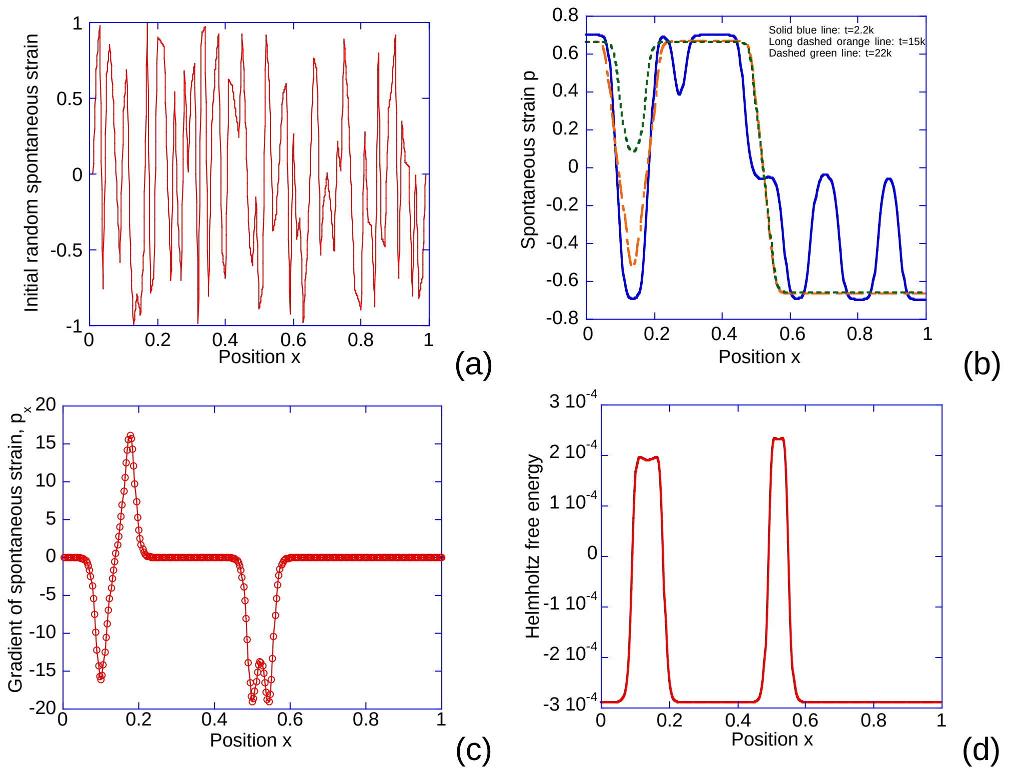

Fig. 2 (a) Initial random distribution of the spontaneous strain p, (b) time evolution of p, (c) gradient of p at equilibrium, and (d) Helmholtz free energy at equilibrium.

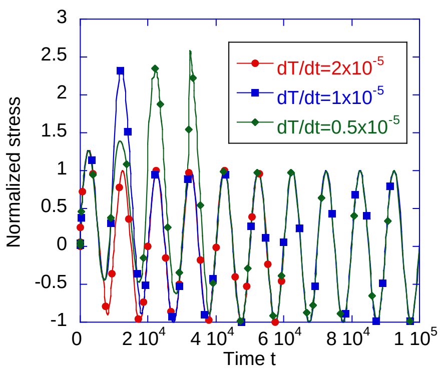

Fig. 3 Stress responses of the 1D system under sinusoidal displacement control with thermal cycling.

3. CONCLUSIONS

In this study, phase transformation kinetics is investigated through time evolution of polarization and other field variables reveals the behavior of the system at different time stages. When under sinusoidal mechanical loading, small temperature loading rates prolong the phase transition effects, consistent with experimental findings, as well as softening anomalies. Our findings here may shed light on further research about negative-stiffness (ferroelastic) composites for their extreme properties and deformation mechanisms.

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