NAMT
98-001

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Research Report No. 98-NA-001

May, 1998

Sponsors

U.S. Army Research Office
Research Triangle Park
NC 27709

National Science Foundation
4201 Wilson Boulevard
Arllington, VA 22230

Proceeding Materials Research Society
Spring 1998

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ABSTRACT

Metastable systems pose significant problems in both analysis and simulation. We discuss here the evolution of microstructure in a shape-memory alloy where energetic contributions from disparate scales play determining roles. This is a challenge for modelling since the finest length scales cannot be 'seen' at macroscopic level. We then provide a mechanism for kinetics that gives a different notion metastability.

INTRODUCTION

We address here modelling the evolution of microstructure in a mosaic of twinned and compound twinned lamellar structures in shape memory CuAlNi, Abeyartne, Chu and James [1]. In this system there is an alternation between two martensitic variants under loading in which the material selects a succession of fine phase intermediate configurations. At each value of the load, the system is in equilibrium save for small regions near mosaic interface, and, during the process, one variant grows at the expense of the other. Although the entire system has the appearance of a succession of equilibria, there is hysteresis in the macroscopic volume fractions of the variants. Thus the system traverses a succession of metastable states. The origin of this behavior is the small amount of energy stored in the mosaic interfaces. These are, however, spatially localized. So this system exhibits metastable behavior across disparate length scales and is an excellent candidate for methods of multiscale analysis. This is a report on joint work with Richard Jordan and Felix Otto, [2],[3],[4],[5].

A typical problem of multiscale analysis proceeds by the introduction of a parameter in a continuum or phenomenological description of the system under discussion and subsequent passage to the limit as this parameter tends to zero or to infinity. Or, as a sort of inverse to this approach, the behavior of the system at a small scale may be assumed and a limit process analogous to an infinite parallel circuit attempted to obtain an effective macroscopic description, [6]. These methods are very useful when the physics of the system is in the realm of continuum mechanics at all the scales and, importantly, when a clear idea of the energy of the system is available for its complete operating range. For example the effective stress tensor of a polycrystalline material may be obtained by such considerations, but these methods begin to fail when properties involving the grain boundaries are sought. A chemical system involving huge numbers of particles behaving in some random fashion, according to a Langevin Equation, may be understood at macroscopic level by means of its distribution function, the solution of a Fokker-Planck Equation. In this case, the nature of the physics itself has changed, since concern is now directed to evolution of the distribution function. Even here, however, there is little hint about the appropriate dynamics of the system at the macroscopic scale, since knowledge of the state of the system at each time does not of itself provide a way to identify nearby states.

Here we wish to consider a somewhat different approach, involving several coarse graining mechanisms, and seek to shed some insight on [1]. The principal device we employ is a representation of local spatial averages of a configuration in terms of a distribution, a measure

called the Young Measure [7],[8]. Although a configuration of a nonlinear material may appear macroscopically as nearly homogeneous, it may consist on interrogation to have complex microstructure, for example of arrangements of fine phase laminates or defect structures. The Young Measure is especially useful in this situation, cf. [8] and [7],[6] for particular applications. Our interpretation of the kinetics of the system will be in terms of how this measure changes and leads to a new interpretation of its metastability.

1. CONSTRAINED THEORY AND COARSE GRAINING

The macroscopic energy of a configuration of the material subjected to a dead load is given by

$$E = \int_\Omega (W(\nabla y) - S\cdot\nabla y)\, dx \ , \tag{1.1}$$

where $y: \Omega \to \mathbf{R}^n$ $(n = 2 \text{ or } 3)$ is the deformation, W is the Helmholtz free energy, and S is the load. The key feature of this energy W is that the symmetries of the lattice imply it has potential wells: W is minimized on a set of copies of $SO(3)$, e.g., $\Sigma = SO(3)U_1 \cup \dots \cup SO(3)U_N$, where the U_k are explicit matrices that emerge from theory, [7],[9],[10]. Equilibrium configurations are sought as minimizers of (1.1). Neglected at this scale, for example, are surface energies, higher gradients, or energies of internal boundaries. The energy is lumpy and rough owing to the complex crystallography of the material. When equilibria are sought, minimizing sequences tend to populate several wells leading to highly oscillatory sequences that converge only weakly.

We turn our attention to the distribution of this population of values, which gives rise to the Young measure. In this context, our measure is a family $\nu = (\nu_x)_{x\in\Omega}$ of probability measures generated by a sequence of deformations

$$\begin{aligned} &y^k: \Omega \to \mathbf{R}^n,\ \nabla y^k \overset{*}{\longrightarrow} \nabla y \text{ in } L^\infty, \text{ such that for any continuous } f, \\ &f(\nabla y^k) \overset{*}{\longrightarrow} \bar{f} \text{ in } L^\infty,\ \bar{f}(x) = \int_M f(A)\, d\nu_x(A) \text{ in } \Omega \text{ a.e.}, \end{aligned} \tag{1.2}$$

where M denotes matrices. We may interpret y^k as a snapshot of the deformation at scale proportional to $1/k$. The energy and deformation gradient of a configuration subjected to a constant dead load S now has the expression

$$E = \int_\Omega \int_M (W(A) - S\cdot A)\, d\nu_x(A) \quad \text{and} \quad \nabla y(x) = \int_M A\, d\nu_x(A). \tag{1.3}$$

The constrained theory consists in identifying a set of admissible measures for the system, typically a subset of ν with $\operatorname{supp}\nu \subset \Sigma$. In CuAlNi there are six potential wells comprising this set, they are described in [1],[7],[9]. In our model problem, a further constraint arises by optimizing E over lamellar structures which populate two wells, say $SO(3)U_1$ and $SO(3)U_2$ subject to a biaxial load S with $Se_3 = 0$. The wells U_1 and U_2 have e_3 as a common axis perpendicular to the plane of the sample, so from this point on, we think of our system as being two dimensional. The result of this process is that we may restrict our attention to a one parameter family and homogeneous deformation gradient

$$\nu^{(\xi)} = (1-\xi)\delta_{M_1(\xi)} + \xi\delta_{M_2(\xi)},\ M_i(\xi) \in SO(3)U_i,\ 0 \le \xi \le 1, \tag{1.4}$$

$$F(\xi) = (1-\xi)M_1(\xi) + \xi M_2(\xi),\ M_2(\xi) - M_1(\xi) = a(\xi)\otimes n,\ |n| = 1, \qquad (1.5)$$

and subject to the fine phase coherence property (rank-one condition) with respect to the second laminate system where it encounters U_2,

$$F(\xi) = U_2(1 + b(\xi)\otimes m(\xi)),\ |m(\xi)| = 1. \qquad (1.6)$$

The energy per unit area at ξ is given by a function

$$E_{loading} = \psi_{macro}(\xi,S) = -\int_M S\cdot A\, dv_x(A) = -F(\xi)\cdot S,\ 0 \le \xi \le 1, \qquad (1.7)$$

which is nearly linear, or even concave, [1]. This is the macroscopic contribution, but note that owing to the optimization process, which involves varying over rotations, it is a function of the Young measure through the volume fraction ξ.

The second and third contributions to the energy cannot be seen by the average bulk deformation $F(\xi)$ because they are regulated by finer scales. However, we can express them in terms of the Young Measure. Here we summarize our results. In the mesoscale regime, there is some stress near the interface between the fine phase laminate given by $F(\xi)$ and U_2, say $x\cdot m(\xi) = 0$, because it is fine phase coherent in the sense that (1.6) holds, but it is not exactly coherent in the sense that $M_1(\xi) - U_2 \neq$ rank 1 and $M_2(\xi) - U_2 \neq$ rank 1. This term may be written, after some calculation for an appropriate f in (1.2),

$$E_{transition\ layer} = \psi_{meso}(\xi) = c(\xi - \tfrac{1}{2})^2 + c_0, \qquad (1.8)$$

The contributions (1.7) and (1.8) are derived in [1].

Fine scale oscillations are implicated in the dynamical behavior of the sample and this will account for the "wiggles" in the analysis of [1]. We suggest that their origin arises from small distortions of the lattice near the interface $x\cdot m(\xi) = 0$. By idealizing this situation as a regular lattice to one side of a line, cut at a prescribed slope α, we may obtain a crude notion of the nature of this contribution. (1.6) implies that α is proportional to ξ. In general, the format of embedded atom potentials may be applied, [11],[12]. We obtain here, where δ and h are lattice parameters, $1/K$ is a scale factor, and $\langle\ \rangle$ denotes a periodic function of period 1,

$$\psi_{micro}(\xi) = \Psi\Big(\frac{1}{K}\sum_1^K f(\delta\langle\frac{\alpha h}{\delta}k\rangle)\Big) \qquad (1.9)$$

For a special choice of Ψ and f,

$$\psi_{micro}(\xi) = \varepsilon\,\psi_0(\frac{\xi}{\varepsilon}),\qquad \varepsilon \approx 1/K, \qquad (1.10)$$

which is the ansatz of [1]. We thus arrive at an idealized effective energy per unit interface length of the form

$$\psi_\varepsilon(\xi) = \psi_{macro}(\xi,S) + \psi_{meso}(\xi) + \varepsilon\,\psi_0(\frac{\xi}{\varepsilon}). \qquad (1.11)$$

2. Evolution of the Microstructure and Fokker-Planck Dynamics

The sample is subjected to a loading program $S = S(t)$. The most straight forward assumption about its motion is the driving force equation

$$\frac{d\xi}{dt} = -\mu\frac{\partial\psi_\varepsilon}{\partial\xi},\quad t > 0. \qquad (2.1)$$

(We take $\mu = 1$ for convenience in the sequel.) To solve this equation iteratively, e.g., by backward-Euler, given $\xi^{(k-1)}$, determine $\xi^{(k)}$ the solution of

$$\frac{1}{\tau}(\xi - \xi^{(k-1)}) = -\psi_\varepsilon'(\xi),$$

which is the same as asking for the ξ such that

$$\frac{1}{2\tau}(\xi - \xi^{(k-1)})^2 + \psi_\varepsilon(\xi) = \min. \qquad (2.2)$$

The above is an expression of competition between the distance of the nearby states $\xi^{(k-1)}$, $\xi^{(k)}$ and the energy $\psi_\varepsilon(\xi^{(k)})$. This suggests a second coarse graining in terms of the distributions of the volume fractions. Given a distribution $\rho^{(k-1)}$ of $\xi^{(k-1)}$ we should seek a distribution $\rho^{(k)}$ of $\xi^{(k)}$ in such a way that

$$\frac{1}{2\tau}\int_R\int_R(\xi-\eta)^2\,d\rho(\xi,\eta) + \int_R \psi_\varepsilon\,\rho\,d\xi + \sigma\int_R \rho\log\rho\,d\xi = \min \qquad (2.3),$$

where ρ is a joint distribution of $\rho^{(k-1)}$ and ρ and the last term represents a configurational entropy. The first term above is related to the Wasserstein metric and defines a weak toplogy on the distributions $f(\xi)\,d\xi$. The second and third terms represent the free energy of the system. This determines the kinetics and from it we understand metastability as a competition between distance and energy. We may calculate and Euler Equation for this process and it turns out that as $\tau\to 0$, the sequence of solutions $(\rho^{(k)})$ converges to the solution of the Fokker-Planck Equation

$$\frac{\partial\rho}{\partial t} = \sigma\frac{\partial^2\rho}{\partial\xi^2} + \frac{\partial}{\partial\xi}(\psi_\varepsilon'\rho),\quad -\infty < \xi < \infty,\ t > 0, \qquad (2.4)$$

We may resolve the path of the motion by computing the solution of (2.4), either analytically or by a numerical technique of our choice.

3. Sample Simulation: A Creep Test

Consider a creep test. Here the material is held in a position, loaded, and then released. Set

$$\psi(\xi) = \frac{1}{2}(\xi - \tfrac{1}{2})^2 \quad\text{and}\quad \psi_\varepsilon(\xi) = \frac{1}{2}(\xi-\tfrac{1}{2})^2 + \varepsilon\psi_0(\frac{\xi}{\varepsilon}),\ |\psi_0'| \le a. \qquad (3.1)$$

In the creep test, we solve (2.4) for ψ and ψ_ε with ρ_0 concentrated near $\xi = 0$. We used an explicit finite difference scheme to calculate the solution. The averages

$$\langle \xi \rangle_t = \int_R \xi \rho \, d\xi \quad \text{and} \quad \langle \xi_\varepsilon \rangle_t = \int_R \xi \rho_\varepsilon \, d\xi \tag{3.2}$$

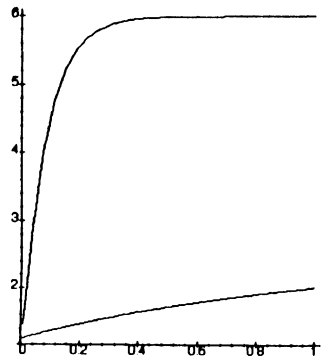

Fig. 1. The results of a creep test, showing the mean values $\langle \xi \rangle_t$, upper curve, and $\langle \xi_\varepsilon \rangle_t$, lower curve. $\langle \xi \rangle_t$ has reached its stationary state by $t = 0.45$.

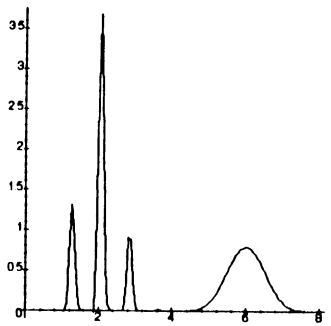

Fig. 2. Final distributions ρ_ε, on the left, and ρ, on the right at $t = 1$ of (2.4).

should display the quite different behavior: $\langle \xi \rangle_t$ should saturate near its stationary value $\frac{1}{2}$ quickly while $\langle \xi_\varepsilon \rangle_t$ should advance slowly. This is indeed the case in the example shown in Figure 1, (which was computed, however, with a scale for ξ whose saturation value is 6). The densities ρ and ρ_ε at the end of the simulation are shown in Figure 2. ρ in fact is essentially the Gibbs distribution. Hence, we believe that Fokker-Planck dynamics can describe metastable systems governed by competition in weak topologies. There are, of course, other dynamical mechanisms that describe other situations.

Conclusions

We have reviewed a metastable system characterized by a reversible transforming microstructure with

(a) a heirarchy of scales analysis of energetics based on a coarse graining that employs statistics of the deformation (the Young Measure or other device) and

(b) the interpretation of metastable evolution in terms of a competition between energy and nearness of successive distributions in terms of a second coarse graining, resulting in a Fokker-Planck type equation.

Acknowledgements

The authors acknowldege the close collaboration of Richard James and Shlomo Ta'asan. This research was supported by the ARO and the NSF.

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