Explicit kinetic relation from "first principles"

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Abstract

We study a fully inertial discrete model of a martensitic phase transition which takes into account interactions of first and second nearest neighbors. Although the model is Hamiltonian at the *microscale*, it generates a nontrivial *macroscopic* relation between the velocity of the martensitic phase boundary and the conjugate configurational force. The apparent dissipation is due to the induced radiation of lattice waves carrying energy away from the front.

Introduction

The fact that a nonzero configurational force is required to sustain a martensitic phase transition reflects inability of the classical continuum elasticity to describe dissipative phenomena inside the transition front where discreteness of the underlying crystal structure cannot be neglected. We recall that in continuum theory a phase boundary can move without friction. At the same time its motion in a lattice can be compared to that of a particle placed in a wiggly (Peierls-Nabarro) landscape: the oscillations of the velocity then lead to the energy transfer from macro to microscale [14]. At continuum level the emitted short-length lattice waves are invisible, and the radiation is perceived as energy dissipation. Since the rate of energy release at the macroscale remains unspecified, in order to close the system of equations at the macrolevel, one needs to supplement the conservative continuum equations with the dissipative kinetic relation on the moving discontinuity [10, 11]. In this paper we consider the simplest nonlocal discrete model of a martensitic phase boundary allowing one to find the unknown energy release rate explicitly. Following some previous work in fracture [7, 8] and plasticity [1, 3, 4] we use a biparabolic ansatz for the free energy and construct an explicit solution of the discrete problem. We emphasize that our only input information concerns the elasticities of the

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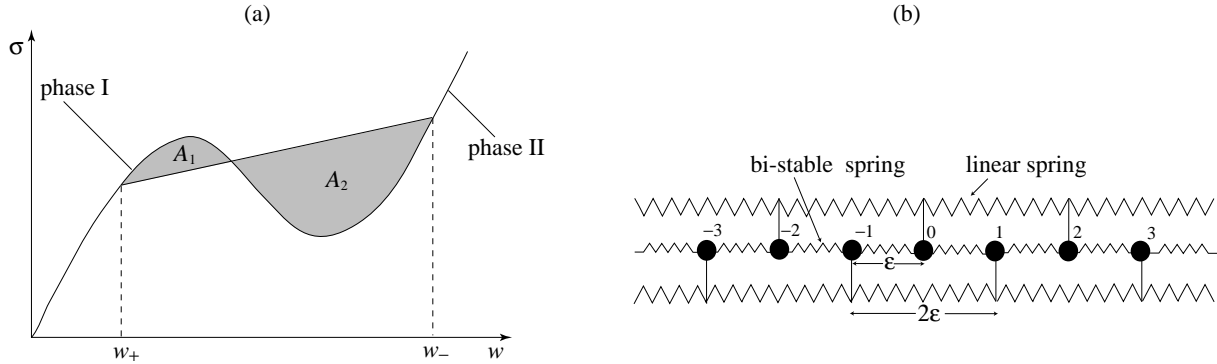[†]Department of Mathematics, University of Pittsburgh, Pittsburgh, PA 15206, aav4@math.pitt.edu

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Figure 1: (a) The macroscopic stress-strain law and the Rayleigh line for a subsonic phase boundary. The difference $A_2 - A_1$ between the shaded areas is the configurational force G. (b) The discrete microstructure with nearest and next-to-nearest neighbor interactions.

constitutive elements, and hence the resulting kinetic relation can be considered of the "first principles" type.

1   Continuum Model

Consider an isothermal motion of an infinite homogeneous bar with a unit cross-section. Let $u(x,t)$ be the displacement of a reference point x at time t. Then strain and velocity fields are given by $w = u_x(x,t)$ and $v = u_t(x,t)$, respectively. The balances of mass and linear momentum are $v_x = w_t$ and $\rho v_t = (\sigma(w))_x$, where the function $\sigma(w)$ specifies the stress-strain relation. To model martensitic phase transitions, we follow [2] and assume that $\sigma(w)$ is non-monotone as shown in Figure 1a. The two monotonicity regions where $\sigma'(w) > 0$ will be associated with material phases I and II. Suppose now that an isolated strain discontinuity propagates along the bar with constant velocity V. On the discontinuity the balance laws reduce to the Rankine-Hugoniot jump conditions

$$\rho V^2 [\![w]\!] = [\![\sigma]\!], \quad \rho V [\![v]\!] = -[\![\sigma]\!], \tag{1}$$

where $[\![f]\!] \equiv f_+ - f_-$ denotes the jump. Conditions (1) must be supplemented by the entropy inequality $\mathcal{R} = GV \geq 0$, where

$$G = [\![\phi]\!] - \{\sigma\}[\![w]\!] \tag{2}$$

is the associated configurational force. Here $\{\sigma\} = (\sigma_+ + \sigma_-)/2$. Given V and the state (v_+, w_+) in front of the moving discontinuity, one can use (1) to determine the state (v_-, w_-) behind. In particular, $(1)_1$ implies that $w_\pm$ lie on the intersection of the

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curve $\sigma(w)$ and the Rayleigh line with the slope ρV^2, as shown in Figure 1a. To satisfy the entropy inequality it is sufficient to require that the difference between the areas A_2 and A_1 shown in Figure 1a is nonnegative. It is not hard to see that the macroscopic jump conditions do not provide enough information to specify the velocity of the phase boundary V uniquely.

Although the difficulty with finding V does not arise in the case of supersonic shock waves, it is essential in the case of subsonic phase boundaries, where additional jump condition controlling the rate of dissipation must be provided to ensure that the continuum problem is well posed [6, 12]. The corresponding closing kinetic relation in the form $G = G(V)$ can be either postulated as a phenomenological constitutive relation (e.g. [10, 11]) or derived from a regularized continuum model which usually includes dissipative as well as dispersive terms (e.g. [5, 10]). Below we take a different approach and derive the closing relation from a discrete lattice model represented by an infinite system of coupled ordinary differential equations.

2 Discrete model

Consider a chain of particles connected to their nearest neighbors (NN) and next-to-nearest neighbors (NNN) by elastic springs, as shown in Figure 1b. In the undeformed configuration the NN and NNN springs have length ε and 2ε, respectively. Let $u_n(t)$, $-\infty < n < \infty$, denote the displacement of nth particle at time t with respect to the reference configuration. In terms of the strain variables $w_n = (u_n - u_{n-1})/\varepsilon$ the dynamic equations take the form

$$m\ddot{w}_n = \phi'_{\text{NN}}(w_{n+1}) - 2\phi'_{\text{NN}}(w_n) + \phi'_{\text{NN}}(w_{n-1}) + \gamma(w_{n+2} - 2w_n + w_{n-2}). \tag{3}$$

Here ϕ_{NN} is the nonlinear and nonconvex NN potential, while the NNN interactions are assumed to be linear: $\phi'_{\text{NNN}}(w) = 2\gamma w$. We seek solutions of (3) in the form of a traveling wave moving with the velocity V and connecting two states in different phases. Let $x = n\varepsilon - Vt$ and assume that

$$u_n(t) = u(x), \qquad w_n(t) = w(x) = [u(x) - u(x - \varepsilon)]/\varepsilon \tag{4}$$

The system (3) can now be replaced by a single nonlinear advance-delay differential equation for $w(x)$:

$$\begin{aligned} mV^2 w'' &= \phi'_{\text{NN}}(w(x + \varepsilon)) - 2\phi'_{\text{NN}}(w(x)) + \phi'_{\text{NN}}(w(x - \varepsilon)) \\ &\quad + \gamma(w(x + 2\varepsilon) - 2w(x) + w(x - 2\varepsilon)). \end{aligned} \tag{5}$$

The states at $x = \pm\infty$ must correspond to their macroscopic limits

$$w(x) \to w_\pm \quad \text{as } x \to \pm\infty. \tag{6}$$

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Since we expect emission of elastic waves, the limits in (6) must be understood in the weak sense only.

In order to obtain analytical solution of the discrete problem, we choose NN potential to be biparabolic and symmetric so that $\phi'_{\text{NN}}(w) = K(w - a\theta(w - w_c))$, where $\theta(x)$ is a unit step function. Assume that all springs in the region $x > 0$ are in phase I, while all springs with $x < 0$ are in phase II. Then in nondimensional variables equation (5) can be written as

$$V^2 w'' - w(x+1) + 2w(x) - w(x-1) - \frac{\beta}{4}(w(x+2) - 2w(x)$$
$$+ w(x-2)) = -\theta(-x-1) + 2\theta(-x) - \theta(1-x), \tag{7}$$

where $\beta = 4\gamma/K$ is the main nondimensional parameter of the problem. Observe that Eq. (7) is linear in $x < 0$ and $x > 0$ so that the nonlinearity is hidden in the switching condition

$$w(0) = w_c \tag{8}$$

and in the constraints

$$w(x) < w_c \quad \text{for } x > 0, \qquad w(x) > w_c \quad \text{for } x < 0 \tag{9}$$

ensuring that the springs are in proper phases. The problem now reduces to solving (7) subject to (6), (8) and (9). We remark that a related discrete problem with $\beta = 0$ (no NNN interactions) was previously considered in [8, 9].

3 Solution of the discrete problem

Equation (7) can be solved by standard Fourier transform (see [13] for details) yielding

$$w(x) = \begin{cases} w_- + \sum\limits_{k \in M^-} \dfrac{4\sin^2(k/2)e^{ikx}}{kL'(k)} & x < 0 \\ w_- - \dfrac{1}{1 + \beta - V^2} - \sum\limits_{k \in M^+} \dfrac{4\sin^2(k/2)e^{ikx}}{kL'(k)} & x > 0, \end{cases} \tag{10}$$

where

$$L(k) = 4\sin^2(k/2) + \beta \sin^2 k - V^2 k^2$$

and

$$M^\pm = \{k : L(k) = 0, \ \{Imk \gtrless 0\} \cup \{Imk = 0, \ kL'(k) \gtrless 0\}.$$

The solution can be viewed as a homogeneous state superimposed with the combination of plane waves with phase velocity V and wave numbers given by the zeroes of $L(k)$. In

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particular, there is a finite number of real roots of $L(k) = 0$ corresponding to radiative modes. To obtain (10), we applied the radiation conditions [1, 7] requiring that all radiative modes with group velocities V_g higher than the interface velocity V appear in front of the moving phase boundary ($x > 0$), while all radiative modes with $V_g < V$ appear behind the front. Since

$$V_g = V + \frac{L'(k)}{2Vk},$$

the relevant radiative modes ahead (behind) the interface must satisfy $kL'(k) > 0$ (< 0).

Equations (10) imply that the limiting states are related by

$$w_+ = w_- - \frac{1}{1 + \beta - V^2},$$

which is exactly the macroscopic Rankine-Hugoniot condition $(1)_1$. The switching condition (8) implies that

$$w_\pm = w_c \mp \frac{1}{2(1 + \beta - V^2)} + \sum_{k \in N^\pm_{\text{pos}}} \frac{4\sin^2(k/2)}{|kL'(k)|}, \tag{11}$$

where $N^\pm = \{k : L(k) = 0,\ Imk = 0, kL'(k) \gtrless 0\}$. Since both $L(k)$ and $N^\pm$ depend explicitly on V, Eq. (11) provides two additional relations between the velocity of the moving interface and the strains at infinity; one of them is equivalent to $(1)_1$ while the other one generates a nontrivial kinetic relation. To recover the second Rankine-Hugoniot condition $(1)_2$, we recall that given the self-similar ansatz (4), the strain and velocity fields are related through $v(x) - v(x-1) = w'(x)$. Since the right hand side of the latter equation is known explicitly (see (10)), we can again use the Fourier transform to show that the difference between the average velocities at infinity satisfies $v_+ - v_- = V/(1 + \beta - V^2)$, This is exactly our macroscopic jump condition $(1)_2$.

4   Kinetic relation

Consider the global energy balance in the discrete model

$$\frac{d}{dt}\left\{ \sum_{n=-\infty}^{\infty} \left[\frac{v_n^2}{2} + \phi_{\text{NN}}(w_n) + \frac{\beta}{2}\left(\frac{w_n + w_{n+1}}{2} \right)^2 \right] \right\} = F_n v_n |_{n=-\infty}^{n=\infty}, \tag{12}$$

where $F_n = \phi'_{\text{NN}}(w_n) + \frac{\beta}{4}(w_{n-1} + 2w_n + w_{n+1})$ is the total force acting on the nth particle from the left. Since at infinity our solution tends to the homogeneous state plus linear oscillations we use asymptotic orthogonality of the modes and write

$$\langle F_n v_n |_{n=-\infty}^{n=\infty} \rangle = \mathcal{P} + \mathcal{P}_0,$$

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where $\langle \cdot \rangle$ denotes the averaging over sufficiently large period, $\mathcal{P} = \sigma_+ v_+ - \sigma_- v_-$ is the macroscopic power supply at $\pm\infty$ and $\mathcal{P}_0$ is the energy carried away by the microscopic lattice waves:

$$-\mathcal{P}_0 = \sum_{k \in N^+} \langle \mathcal{G}_k \rangle_+ (V_g - V) + \sum_{k \in N^-} \langle \mathcal{G}_k \rangle_- (V - V_g). \qquad (13)$$

Here $\mathcal{G}_k$ is the sum of kinetic and potential energies per particle carried by the mode k. The average energy density carried by the mode k can be computed from $\langle \mathcal{G}_k \rangle = \langle \mathcal{G} - \mathcal{G}_0 \rangle_k$, where $\mathcal{G}(x)$ is the total energy per particle and $\mathcal{G}_0$ is the energy of the limiting homogeneous states. The calculation yields [13]

$$\langle \mathcal{G}_k \rangle_\pm = \frac{8V^2 \sin^2(k/2)}{(L'(k))^2}$$

for the the average energy density carried by the radiative wave with $k \in N^\pm_{\mathrm{pos}} = \{k \in N^\pm : k > 0\}$. Substituting these explicit relations into (13) and observing that $\mathcal{R} = GV = -\mathcal{P}_0$, we obtain the desired expression for the driving force:

$$G = 4 \sum_{k \in N^\pm_{\mathrm{pos}}} \frac{\sin^2(k/2)}{|kL'(k)|}. \qquad (14)$$

Since both $L(k)$ and $N^\pm$ are known functions of V, Eq. (14) yields an explicit kinetic relation (see also 11).

Alternatively, we could compute the driving force G by using Eq. (2) for the continuum macromodel. Observe that the macroscopic energy density $\phi(w)$ is related to its microscopic counterparts via

$$\phi(w) = \frac{1}{2}(1 + \beta)w^2 - \theta(w - w_c)(w - w_c).$$

By substituting this relation into (2) and using (11), we obtain

$$G = \frac{1}{2}(w_- + w_+) - w_c = 4 \sum_{k \in N^\pm_{\mathrm{pos}}} \frac{\sin^2(k/2)}{|kL'(k)|},$$

which coincides with (14). This confirms that the macroscopic energy release rate is consistent with the microscopic account of dissipation.

To compute the resulting kinetic relation we need to find at each V all positive real zeroes of $L(k)$. The typical function $V(k)$ is plotted in Figure 2a. It possesses an infinite number of local maxima V_i^r (resonance velocities) where $L'(k) = 0$ and the sums in (10) and (14) diverge. These resonances are symmetry-related and disappear when the
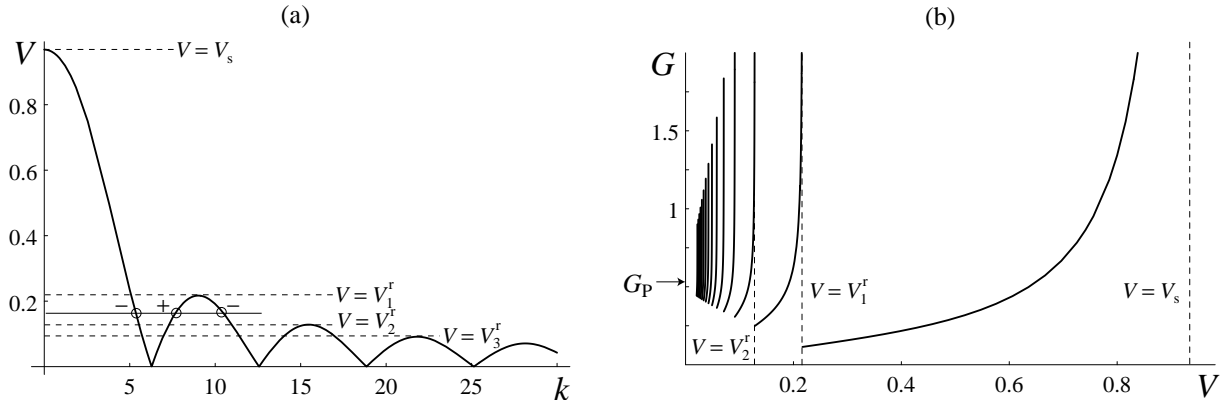
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Figure 2: (a) Real wave numbers k corresponding to a given interface velocity V with "+" and "−" denoting the sign of $kL'(k)$. Also marked are the resonance velocities V_i^r. (b) Mobility curves $G(V)$. The entire region around the resonances should be excluded. In both graphs $\beta = -1/8$.

curvatures of the energy wells are different [3]. Two limiting cases, $V \to 0$ and $V \to V_s$, where $V_s = \sqrt{1+\beta}$ is the macroscopic sound velocity, deserve particular attention. In the zero-velocity limit we obtain [13]

$$ G(0) = \frac{1}{2\sqrt{1+\beta}} = G_{\mathrm{P}}, $$

which coincides with the Peierls force computed in [14]. The limit $V \to V_s$ depends on β. Assume for determinacy that $-1/4 < \beta \le 0$. Then one can show that for $V \to V_s$ the only relevant positive real root $k \in N_{\mathrm{pos}}^-(V)$ tends to zero and since in this limit

$$ G = \frac{6}{(1+4\beta)k^2} + \frac{44\beta - 1}{10(1+4\beta)^2} + O(k^2), $$

we obtain that $G(V) \to \infty$.

In the intermediate range $0 < V < V_s$ the kinetic relation can be obtained numerically by computing the sets $N_{\mathrm{pos}}^\pm(V)$. Figure 2b shows the typical mobility curves $G(V)$ at $\beta = -1/8$. As expected, in the small-velocity range $0 < V \le V_1^r$ there is an accumulation of resonances. It can be shown [13] that the corresponding traveling wave solution are not admissible because they violate the condition (9). In this range of average velocities the interface motion may be of a more complex nature, for instance, stick-slip.

References

[1] W. Atkinson and N. Cabrera. Motion of a Frenkel-Kontorova dislocation in a one-dimensional crystal. *Phys. Rev.*, 138(3A):763–766, 1965.

[2] J.L. Ericksen. Equilibrium of bars. *J. Elast.*, 5:191–202, 1975.

[3] O. Kresse and L. Truskinovsky. Hamiltonian dynamics of a driven asymmetric kinks: an exact solution. *Physica D*, 2003. Submitted.

[4] O. Kresse and L. Truskinovsky. Mobility of lattice defects: discrete and continuum approaches. *J. Mech. Phys. Solids*, 51(7):1305–1332, 2003.

[5] S.-C. Ngan and L. Truskinovsky. Thermal trapping and kinetics of martensitic phase boundaries. *J. Mech. Phys. Solids*, 47:141–172, 1999.

[6] S.-C. Ngan and L. Truskinovsky. Thermoelastic aspects of nucleation in solids. *J. Mech. Phys. Solids*, 50:1193–1229, 2002.

[7] L. I. Slepyan. Dynamics of a crack in a lattice. *Sov. Phys. Dokl.*, 26(5):538–540, 1981.

[8] L. I. Slepyan. Feeding and dissipative waves in fracture and phase transition II. Phase-transition waves. *J. Mech. Phys. Solids*, 49:513–550, 2001.

[9] L. I. Slepyan and L. V. Troyankina. Fracture wave in a chain structure. *J. Appl. Mech. Techn. Phys.*, 25(6):921–927, 1984.

[10] L. Truskinovsky. Equilibrium interphase boundaries. *Sov. Phys. Dokl.*, 27:306–331, 1982.

[11] L. Truskinovsky. Dynamics of nonequilibrium phase boundaries in a heat conducting elastic medium. *J. Appl. Math. Mech.*, 51:777–784, 1987.

[12] L. Truskinovsky. Kinks versus shocks. In *Shock Induced Transitions and Phase Structures in General Media*, pages 185–229. Springer-Verlag, New York, 1993.

[13] L. Truskinovsky and A. Vainchtein. 2003. In preparation.

[14] L. Truskinovsky and A. Vainchtein. Peierls-Nabarro landscape for martensitic phase transitions. *Phys. Rev. B*, 67:172103, 2003.