Peierls-Nabarro landscape for martensitic phase transitions

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Abstract

We propose a simple one-dimensional model which can be used to reconstruct the Peierls-Nabarro energy landscape and compute the limits of lattice trapping for martensitic phase transitions. The model represents a nontrivial analog of the discrete Frenkel-Kontorova model. We find the explicit expression for the critical driving force which sets phase boundaries in motion and delimits the width of the rate-independent hysteresis. The theory is applied to β-martensitic phase transition in Cu-Al-Ni alloy.

Rate-independent hysteresis is commonly observed in materials undergoing martensitic phase transitions, e.g. Ag-Cd [1], In-Tl [2], Cu-Al-Ni [3, 4] and Ni-Ti [5, 6]. When subjected to a quasistatic tensile loading, these materials deform elastically until the load reaches a critical value. At the critical load one or several phase boundaries nucleate and propagate through the specimen. Upon unloading the reverse transformation takes place at a lower critical load. Quantitative prediction of the width of the resulting quasistatic hysteresis and the associated kinetics of the moving interfaces represents an important challenge for the theory [7, 8].

While it is well understood that the rate-independent hysteresis in martensites reflects the presence of multiple metastable configurations, the physical origin of the critical load has been a subject of rather different theories emphasizing: disorder [9], elastic incompatibility [10], surface energy [11] and material discreteness [12]. The dissipation in these materials is typically attributed to an unavoidable development of fast internal instabilities (Barkhausen jumps) associated with the overall ruggedness of the energy landscape [13, 14, 15]. The martensitic phase boundaries represent highly mobile planar defects of a crystal lattice, and the physical situation is reminiscent of the one in metal plasticity where the analogous carriers of inelastic deformation are linear defects (dislocations). The complex interaction of both kinds of defects with a crystal lattice leads to an intense radiative damping and results in dry-friction type kinetics [16, 17]. Both martensitic phase transformations and plastic flow take place at nearly constant yield load, and in both cases nucleation is typically associated with a small load drop [18, 6]. The driving forces responsible for the release of the transformation-generating defects are known as

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Peach-Koehler force in plasticity [19] and Eshelby force in the theory of martensitic phase transitions [20].

In this paper we follow the pattern of plasticity theory and relate the rate-independent hysteresis in martensites to the presence of the "trapping" domain in the kinetic relations for phase boundaries. In the case of dislocations it has been long realized that there is a clear difference between the ultimate strength of the material in shear and the corresponding Peierls force [21, 19] which is sufficient to release a trapped dislocation and set a plastic deformation in motion. The dislocation is then viewed as a moving point in a Peierls-Nabarro (PN) periodic potential with the valleys representing potential equilibrium locations of the stationary defects. The applied force tilts this landscape until at Peierls force the barriers between the valleys completely disappear. The most detailed computation of the Peierls force for dislocations has been obtained in the framework of the highly idealized discrete Frenkel-Kontorova (FK) model [22].

The goal of the present paper is to develop for martensitic phase boundaries a prototypical one-dimensional model amenable to a detailed analysis and allowing one to reconstruct the fine structure of the PN landscape. The simplest physical model of this type can be represented as a chain of bistable springs [12, 23, 24]; to mimic the three-dimensional nature of the real problem one can add a linear interaction between the next-to-nearest neighbors [25, 26, 27]. The model will then preserve the main features of the FK model: the nonlinearity of the potential for the individual elements and the harmonic coupling.

To be specific, consider an infinite chain of particles linked by bistable nearest-neighbor (NN) springs and harmonic next-to-nearest-neighbor (NNN) springs. Let u_k be the displacement of the kth particle with respect to the unstressed homogeneous reference configuration with spacing ε and $w_k = (u_k - u_{k-1})/\varepsilon$ be the strain in the kth NN spring. Then the total energy of the chain can be written in the form

$$\Psi = \varepsilon \sum_{k=-\infty}^{\infty} [\phi(w_k) - F w_k + \frac{\gamma}{2}(w_{k+1} + w_k)^2]. \tag{1}$$

Here the first term represents the energy of the NN interactions, the second term is the potential of the applied force F, and the third term is the energy of the linear NNN interactions [3].

To model a two-phase material we assume that the NN potential $\phi(w)$ has two wells; to obtain analytical results we further choose it to be bi-parabolic with a piecewise linear derivative

$$\phi'(w) = K(w - a\theta(w - w_c)), \tag{2}$$

Here $\theta(x)$ is a unit step function [4]. The NN springs are in phase I if the strain w is below

[3] This model is different from the FK model because of the plus sign in the last term in (1).

[4] $\theta(x) = 1$ for $x \geq 0$ and $\theta(x) = 0$ for $x < 0$.

the critical value w_c and in phase II otherwise. The other parameters of the potential $\phi(w)$ are the transformation strain a and the elastic modulus $K > 0$ which we take for simplicity to be the same in both phases. The elastic modulus γ of the NNN springs is assumed to be *negative*, as suggested, for example, by molecular models with Lennard-Jones potential [27].

The system of equilibrium equations for the model (1), (2) reads

$$w_k + \frac{\eta}{4}(w_{k+1} + 2w_k + w_{k-1}) = \frac{F}{K} + a\theta(w - w_c), \tag{3}$$

where $\eta = 4\gamma/K$. The trivial solution of these equations is a uniform deformation in one of the phases; for example, the chain is in phase I when $F \le K(1+\eta)w_c$. In what follows we assume that the uniform solution is stable, which in our case ($K > 0$, $\gamma < 0$) translates into the requirement that $-1 < \eta < 0$ [27]. To find a non-trivial solution of (3) with a single phase boundary, we assume that the location of the interface coincides with particle i:

$$w_k \ge w_c,\ k \le i \text{ (phase II)}, \quad w_k \le w_c,\ k > i \text{ (phase I)} \tag{4}$$

The system of nonlinear equilibrium equations (3) can then be rewritten as a system of linear equations with a given right hand side:

$$A_{kl} w_l = F/K + a\theta(i - k). \tag{5}$$

Here A_{kl} is the tridiagonal symmetric matrix which can be easily reconstructed from the left hand side of (3). In addition to the admissibility conditions (4), solutions of (5) must satisfy the boundary conditions at infinity: $w_{-\infty} = (F/K + a)/(1+\eta)$ and $w_{+\infty} = F/(K(1+\eta))$.

The exact solution of the linear problem (5) can be obtained by the standard methods, e.g. Z-transform [28]. We obtain

$$w_k(i) = \frac{F + Ka}{K(1+\eta)} - \frac{a}{1+\eta}\left\{\frac{1-\sqrt{1+\eta}}{2}e^{\lambda(k-i)} + \theta(k-i-1)\left(1 - \frac{\cosh((k-i-1/2)\lambda)}{\cosh(\lambda/2)}\right)\right\}, \tag{6}$$

where $\lambda = 2\ln((1+\sqrt{1+\eta})/\sqrt{|\eta|})$. Using (6), it is easy to show that the constraints (4) are satisfied if and only if the applied force lies in the interval $F_M - F_P \le F \le F_M + F_P$ where $F_M = K(1+\eta)w_c - Ka/2$ is the Maxwell force defined by the equal area construction from the graph of the uniform response $F = K((1+\eta)w - a\theta(w - w_c))$ and

$$F_P = \frac{Ka}{2}\sqrt{1+\eta}. \tag{7}$$

is the Peierls force, whose analog was originally introduced in the theory of dislocations [21, 19]. At $F = F_M + F_P$, the strain in the $(i+1)$th NN spring reaches the critical value

w_c and the single interface solution ceases to exist. At $F = F_M - F_P$, the critical strain is reached in the ith spring. Inside the interval of existence $F_M - F_P < F < F_M + F_P$, which we identify with the region of *lattice trapping*, the solution (6) is (meta)stable due to the positive definiteness of the matrix A_{kl} in (5) guaranteed under our assumptions on elastic moduli.

To reconstruct the PN energy landscape, we need to find the optimal (minimal barrier) connections between the metastable single-interface equilibria. Suppose for determinacy that $F_M < F < F_M + F_P$ and consider the two adjacent equilibrium configurations $w_k(i)$ and $w_k(i+1)$, where the integer argument i marks the location of the phase boundary. In the first of these configurations the $(i+1)$th spring is still in phase I, while in the second this spring has already switched to phase II. In order to move from the first to the second configuration, the system has to follow a non-equilibrium path along which the $(i+1)$th spring changes its phase. Therefore it is natural to choose w_{i+1} as the order parameter and minimize the energy with respect to all other strains w_i with $k \leq i$ and $k \geq i+2$. The necessary conditions for this constrained equilibrium coincide with (5) taken at $k \neq i+1$. The solution of the corresponding equations at $k \leq i$, satisfying the boundary condition at $-\infty$, can be written in the parametric form

$$w_k^-(\nu) = \frac{F + Ka}{K(1+\eta)} - \frac{a(1-\sqrt{1+\eta})e^{\lambda(k-\nu)}}{2(1+\eta)}. \tag{8}$$

Here the parameter ν is defined by the condition $w_{i+1}^-(\nu) = w_{i+1}$, with $i = [\nu]$ (the integer part of ν). In the interval $(i, i+1)$ the function $w_{i+1}^-(\nu)$ monotonically increases with ν from $w_{i+1}^-(i) = w_{i+1}(i)$ to $w_{i+1}^-(i+1) = w_{i+1}(i+1)$. Since w_{i+1} oscillates as the function of i while ν varies monotonically, it is convenient to choose ν as a new order parameter. To complete the construction of the constrained equilibria we need to find $w_k^+(\nu)$ satisfying equilibrium equations for $k \geq i+2$, the boundary condition at $+\infty$ and the continuity condition $w_{i+1}^+(\nu) = w_{i+1}^-(\nu)$. We obtain

$$w_k^+(\nu) = \frac{F}{K(1+\eta)} + \frac{a}{1+\eta} e^{\lambda([\nu]+1-k)} \left(1 - \frac{1-\sqrt{1+\eta}}{2} e^{\lambda([\nu]+1-\nu)}\right). \tag{9}$$

The combination of $w_k^-(\nu)$ taken at $k \leq [\nu]+1$ and $w_k^+(\nu)$ at $k \geq [\nu]+1$ constitutes the desired non-equilibrium solution $w_k(\nu)$. Notice that by construction, the integer values of ν correspond to the metastable configurations $w_k(i)$.

The desired PN potential is now given by the energy along the non-equilibrium path (8), (9). Since the energy (1) is infinite, one can consider the difference between the energy $\Psi(\nu)$ associated with the non-equilibrium path and the energy of one of the metastable equilibria. We define $W(\nu) = \Psi(\nu) - \Psi(0)$ and by substituting (8) and (9) into (1), obtain

$$W(\nu) = \frac{Ka\varepsilon}{1+\eta} \left(\frac{a(1-e^{-\lambda(\nu-[\nu])})^2(1+\sqrt{1+\eta})^2}{8\sqrt{1+\eta}} - \frac{(F-F_M)[\nu]}{K} - \Delta(\nu)\theta(\Delta(\nu)) \right), \tag{10}$$

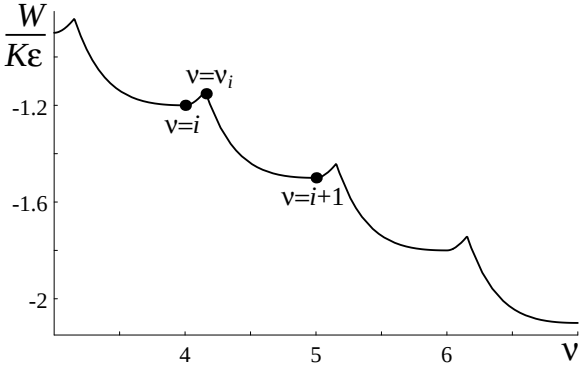

Figure 1: Energy landscape $W(\nu)/(K\varepsilon)$ at $F/K = 0.15$, $\eta = -1/2$, $w_c = a = 1$.

where $\Delta(\nu) = a(1 - (1 + \sqrt{1+\eta})e^{-\lambda(\nu-[\nu])})/2 + (F - F_M)/K$. A typical energy $W(\nu)$ is shown in Figure 1. As expected, the PN landscape exhibits local minima at integer values of ν corresponding to successive metastable locations of the phase boundary. In order to switch from one metastable configuration (say, at $\nu = i$) to the neighboring one (at $\nu = i + 1$), the system needs to climb an energy barrier. In the present piecewise linear setting the maxima of the PN potential (saddle points of the original energy) are represented by the sharp peaks [5]. For each i, the peak is located at $\nu_i \in (i, i + 1)$, which is defined by the condition $w^{\pm}_{i+1}(\nu_i) = w_c$. The energy barrier associated with a peak does not depend on i and is given by the following explicit formula

$$\Delta W = W(\nu_i) - W(i) = \frac{\varepsilon(F_M + F_P - F)^2}{2K(1+\eta)^{3/2}}, \tag{11}$$

The barrier is maximal at Maxwell force $F = F_M$ and vanishes at the upper boundary of the trapping region $F = F_M + F_P$. One can show that if the energy $\phi(w)$ contains a non-degenerate spinodal region, the sharp peaks are replaced by smooth maxima [24].

Another parameter, which plays an important role in the formulation of the kinetic relations for phase boundaries [29], is the *driving force* f represented in the three-dimensional continuum setting by the jump of the normal component of the Eshelby tensor [30]. In our framework $f = (W(i) - W(i+1))/\varepsilon = a(F - F_M)/(1+\eta)$, which is again independent of i. One can see that parameter f measures the degree of tilting of the PN landscape by the external force F. In particular, the driving force equals zero at $F = F_M$ (horizontal PN landscape) and reaches its maximum at $F = F_M + F_P$, when the barriers disappear.

[5] Observe that as a result of non-smoothness of our model, the ith and $(i + 1)$th particles are *not* in equilibrium at the saddle points; instead, they are subjected to forces of equal magnitude $R = Ka/2 - (F - F_M)/(\eta + 1)$ and opposite directions. For an analogous result for the FK model, see R. Hobart, J. Appl. Phys. **36** (1965)

The critical driving force is given by

$$f_P = \frac{aF_P}{1+\eta}. \tag{12}$$

In the limiting case when the NNN interactions are absent the PN landscape was computed in [24], where it was shown that at $\eta = 0$ the minimal barrier path is also associated with a single spring changing phase, while all other springs remain fixed in their equilibrium positions. However, in the NN chain the location of the spring which changes phase is arbitrary. When NNN interactions are taken into account, the degeneracy is removed and the transforming spring is located in front of the phase boundary; in this case not only the strain in the $(i+1)$th spring has to increase and cross the critical value but the surrounding springs must also deform while remaining in their respective phases. The existence of the boundary layer in the NNN chain makes the propagation of the existing phase boundary easier than the nucleation of a new one. As a result, the Peierls force F_P in the NNN model is smaller than the *spinodal force* $F_S = Ka/2$, while in the NN case $F_P = F_S$ [24].

To verify the theory we estimate the strength of NNN interactions from experimental data on kinetics of martensitic phase boundaries and then compare it with an independent estimate based on a simple molecular model of the same solid phase. The formula (7) for the Peierls force implies that

$$\eta = \left(1 + \frac{2(F_P - F_S)}{E\Delta}\right)^2 - 1, \tag{13}$$

where $E = K(1+\eta)$ and $\Delta = a/(\eta+1)$ are the macroscopic elastic modulus and transformation strain, respectively; observe that $Ka = E\Delta$. Recall that the spinodal force F_S measures the half-width of maximal hysteresis. In the bilinear model it is given by $F_S = E\Delta/2$, and if parameters F_P, E and Δ are known from experiment, one can determine parameter η from (13). Note, however, that the assumption about the bilinear character of the force-strain curve for a single spring largely overestimates the maximal hysteresis width [3]. While a more appropriate estimate could in principle be obtained from the model with the cubic force-strain relation, the corresponding discrete model does not lend itself to a simple analytical study. To obtain an improved estimate of η we assume that in the realistic case when F_P is close to F_S the linearized version of (13),

$$\eta \approx \frac{4(F_P - F_S)}{E\Delta}, \tag{14}$$

remains true for the cubic model with the same $E\Delta$. For the cubic interpolation of (2) the spinodal force reduces to $F_S = E\Delta/(6\sqrt{3})$. The Peierls force F_P can then be found

from the formula (12) relating it to the critical driving force f_P, which, in turn, can be obtained from the data on kinetics of martensitic phase boundaries.

To estimate η we use the critical driving force $f_P = 25.26$ MPa reported in [17] for a moving interface between cubic and monoclinic β_1'-phases in a single-crystal Cu-Al-Ni alloy. The other relevant parameters, also provided in [17], are $\Delta = 0.16868$ and $E = 10$ GPa. Substituting these values into (12), (14), we obtain $\eta = -0.0299$, which corresponds to $\gamma = -77.13$ MPa, and $K = 10.3$ GPa.

To check this result, we can alternatively estimate η by assuming that both NN and NNN interactions are governed by the Lennard-Jones potential

$$U(r) = \frac{K\varepsilon}{72}\left[\left(\frac{\varepsilon}{r}\right)^{12} - 2\left(\frac{\varepsilon}{r}\right)^{6}\right], \tag{15}$$

where parameters are selected so that elastic modulus in the potential well located at $r = \varepsilon$ equals K. By linearizing (15) around the unstretched homogeneous state with the spacings $r = \varepsilon$ and $r = 2\varepsilon$, we obtain [27] $\eta = 4U''(2\varepsilon)/U''(\varepsilon)$. This yields $\eta = -0.0177$, which, despite a rather rigid form of the potential (15), is of the same order as the above estimate. With macroscopic elastic modulus $E = 10$ GPa, we obtain $\gamma = -45.1$ MPa, $K = 10.18$ GPa.

We conclude that in spite of its simplicity, the proposed model provides realistic formulae relating macroscopic hysteresis to the microscopic parameters describing interatomic interactions. The natural dynamic extension of this work requires the analysis of the full-scale inertial problem

$$m\varepsilon\ddot{w}_k = \phi'(w_{k+1}) - 2\phi'(w_k) + \phi'(w_{k-1}) + \gamma(w_{k+2} - 2w_k + w_{k-2}). \tag{16}$$

The ruggedness of the PN landscape is then expected to give rise to the stick-slip motion at small averaged velocities and nonzero radiative drag at subsonic and near sonic velocities. The corresponding dynamic studies are currently under way.

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