Frenkel-Kontorova model of propagating ledges on austenite-martensite phase boundaries*

P. Leninpandian and Srikanth Vedantam

Department of Engineering Design, Indian Institute of Technology Madras, Chennai, India 600036

Abstract

Modeling the formation and evolution of microstructure in phase transforming materials presents challenges to traditional continuum mechanics approaches. This is mainly because they do not account for effects arising from the discreteness of the underlying lattice. Such effects can be described by non-classical approaches based on discrete particle models. We study the propagation of an austenite-martensite phase boundary using a Frenkel–Kontorova model. The model is based on a one dimensional chain of atoms on the phase boundary under the influence of a temperature dependent substrate potential. Using this model we derive the kinetic relation as a function of temperature.

Keywords: Frenkel–Kontorova model, phase transitions, kinetic relation, shape memory alloys

1. Introduction

Classical continuum mechanics has made great strides in solving for the deformation and stress in problems involving combinations of mechanical and thermal loads [1]. With the advent of numerical solution methods, problems with extremely complex geometries and boundary conditions are solved relatively accurately [2]. However there are several classes of problems for which classical continuum mechanics faces difficulties in modeling.

Some of the problems which are outside the ambit of classical continuum mechanics are those which involve the nucleation and evolution of defects. Defects may be any localized features involving heterogeneity at smaller length scales – also termed microstructure [3]. Such microstructure is present in almost all materials, but actively evolves during loading in some materials and in certain loading regimes. This evolution of the microstructure affects the overall response of the material and it is important to incorporate the concomitant effects in order to describe the macroscale response. Examples of such evolving defects include the initiation and growth of cracks, shear bands or phase transformations in materials. It is well known that the classical continuum mechanics approach cannot describe these phenomena [4].

Attempts at overcoming this lacuna involve specification of additional constitutive equations on the evolving interfaces [5]. Such constitutive relations are known as kinetic relations which relate the driving force on the defect to its velocity. It is well known that the kinetic relation is strongly dependent on the details of the microstructural features underlying the evolving defects [6].

Non-classical continuum models are based on regularization and employ additional order parameters such as strain gradients or phase field parameters [8–10]. These augmented models possess

*Dedicated to Prof. J. N. Reddy on the occasion of his 75th birthday.

implicit kinetic relations. However, the implicit kinetic relations generally do not account for the detailed microstructural features. In order to model features such as stick-slip kinetics which are affected by the microstructural details, it is necessary to develop relatively complicated phenomenological description of the kinetic parameters in the models [10].

In order to account for the microstructural features in greater detail, other approaches have used atomistic level modeling [11]. It is possible to extract microstructurally informed kinetic relations from such atomistic models and use them along with continuum models. Alternatively, multiscale approaches employ atomistic and continuum approaches in the same domain and solve for the relevant scales simultaneously [12]. However, atomistic scale modeling is computationally prohibitive and provides too much detail. Obtaining macroscopically relevant quantities such as strain [13] or stress [14] from atomistic information also proves to be challenging.

A third possible class of approaches to model the formation and evolution of microstructure is based on discrete particle models [15]. Such models are based on discrete interacting particles at length and time scales relevant to the continuum description. It has been shown that discrete particle models possess features such as radiative damping and lattice trapping which are important to accurate representations of the kinetic relations and, consequently, macroscopic response [16].

There have been several classes of one dimensional discrete models. These approaches are broadly classified as Frenkel-Kontorova (FK) [17] or Fermi-Pasta-Ulam (FPU) [18] type models. While these models do not give quantitative information they do qualitatively indicate the origins of various microscale phenomena at the macroscale. The former was first proposed to study the motion of dislocations in a lattice. The plane in which the dislocation propagates is considered as a chain of particles and the surrounding atoms are taken to provide a sinusoidal substrate potential. Later studies have approximated the substrate to be piecewise parabolic in order to obtain analytical results [19]. This model was adapted to study the motion of ledges on twin boundaries [20]. The latter class of models based on the FPU approach consider non-linear interactions between particles in the one-dimensional chain [21]. These models have also been extended to study phase transformations by considering bi-stable interactions [22].

Generally, the FK models have not considered the effect of temperature. Describing the thermal effects due to atomic vibrations proves to be a challenge. Recently Mahendaran et al [23] developed a discrete particle approach by which the temperature dependent continuum free energy is directly used to derive interparticle interactions in a discrete particle model. Based on this approach, we develop a FK model with a temperature dependent substrate to describe a material undergoing phase transformations. The kinetic relation derived from this FK model is dependent on the temperature through the substrate potential.

We consider a material which undergoes phase transformations from a cubic austenite phase at high temperatures to an orthorhombic martensite phase at low temperatures. The crystallography of such transformations has been calculated in detail [24]. Under certain conditions of the lattice parameters the austenite phase forms an interface with a single variant of martensite. We examine the kinetics of such a boundary using the Frenkel-Kontorova model. Additional insights into the transformation are obtained by considering a quasicontinuum approximation of the problem and analytical solutions of the same [7, 25].

The paper is organized as follows. In Section 2, we outline the essential kinematics and the free energy function appropriate to phase transforming materials. We describe how certain three dimensional problems can be amenable to a one-dimensional description on the phase boundary. Next, in Section 3 we describe the Frenkel-Kontorova model and derive the governing equations for the model. We also consider a simple quasicontinuum approximation of the governing equations.

In Section 4, we present numerical solutions of the governing equations and compare with the analytical traveling wave solution to the quasicontinuum problem. We derive the kinetic relation for this model as a function of temperature.

2. Model

2.1. Kinematics

We begin with a brief description of the kinematics of the austenite–martensite interface. A detailed description of the relevant kinematics can be found in [24] and references therein.

Consider a material which undergoes a phase transformation between a cubic austenite phase and an orthorhombic martensite phase. The martensite phase occurs as six variants. Taking the unstressed austenite to be the reference configuration, the austenite phase is characterized by the deformation gradient tensor $\boldsymbol{F} = \boldsymbol{I}$, the variants of the martensite phase are characterized by $\boldsymbol{F} = \boldsymbol{U}_1, \boldsymbol{U}_2, \ldots, \boldsymbol{U}_6$, where the $\boldsymbol{U}_i$'s are called the Bain stretch tensors. The subscript i is refers to the ith variant.

We consider a coordinate system described by a $\hat{\boldsymbol{e}}_1, \hat{\boldsymbol{e}}_1, \hat{\boldsymbol{e}}_3$ with the unit vectors aligned to the edges of the parent cubic lattice. Then the orthorhombic martensite phase can be described by the stretch tensors for the variants 1 and 2, respectively $\boldsymbol{U}_1$ and $\boldsymbol{U}_2$. In the coordinate system under consideration these take the form

$$\boldsymbol{U}_1 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\gamma-\alpha}{2} & 0 \\ \frac{\gamma-\alpha}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}, \qquad \boldsymbol{U}_2 = \begin{pmatrix} \frac{\alpha+\gamma}{2} & \frac{\alpha-\gamma}{2} & 0 \\ \frac{\alpha-\gamma}{2} & \frac{\alpha+\gamma}{2} & 0 \\ 0 & 0 & \beta \end{pmatrix}, \tag{1}$$

where α, β and γ are transformation stretches which are proportional to the ratios of the lattice constants of the orthorhombic lattice to the side of the cubic parent austenite lattice. The other variants are symmetric representations of the matrices listed above [24].

Under the condition $\gamma > 1, \alpha < 1$ and $\beta = 1$, it is possible for the austenite phase to have a compatible interface with a single variant of martensite. Compatibility of the interface requires that the deformations on the two sides of a phase boundary are rank-one connected. The compatibility condition on the phase boundary with austenite phase on the one side and martensite variant i on the other is

$$\boldsymbol{R}\boldsymbol{U}_i - \boldsymbol{I} = \boldsymbol{b} \otimes \hat{\boldsymbol{m}}, \tag{2}$$

where $\boldsymbol{R}$ is a rotation and $\hat{\boldsymbol{m}}$ is a unit normal to the interface in the reference configuration.

The solutions of the compatibility equation (2) as given by [24] for $i = 1$ are given by

$$\boldsymbol{b}_1 = \frac{1}{\sqrt{2}}\sqrt{\frac{\gamma-\alpha}{\gamma+\alpha}} \begin{pmatrix} \gamma\sqrt{1-\alpha^2} + \kappa\alpha\sqrt{\gamma^2-1} \\ \gamma\sqrt{1-\alpha^2} - \kappa\alpha\sqrt{\gamma^2-1} \\ 0 \end{pmatrix}, \; \hat{\boldsymbol{m}}_1 = \frac{-1}{\sqrt{2(\gamma^2-\alpha^2)}} \begin{pmatrix} \sqrt{1-\alpha^2} + \kappa\sqrt{\gamma^2-1} \\ \sqrt{1-\alpha^2} - \kappa\sqrt{\gamma^2-1} \\ 0 \end{pmatrix} \tag{3}$$

where $\kappa = \pm 1$.

It may be noted that both $\boldsymbol{m}$ and $\boldsymbol{b}$ are in the (x_1, x_2) plane. In fact, if the transformation stretches are chosen such that $\det \boldsymbol{U}_1 = 1$ then it can be shown by simple calculation that $\boldsymbol{b} \cdot \boldsymbol{m} = 0$ and that $\boldsymbol{I} + \boldsymbol{b} \otimes \hat{\boldsymbol{m}}$ is a simple shear deformation. We write $\boldsymbol{b} = \varepsilon\hat{\boldsymbol{b}}$ where ε is the magnitude of the simple shear and $\hat{\boldsymbol{b}}$ is a unit vector in the direction of the shear. The rotation $\boldsymbol{R}$ is about the x_3 axis and the angle is given by $\theta = \arccos\left[(1 + \alpha\gamma)/(\alpha + \gamma)\right]$.

The Cauchy-Born rule relates the continuum deformation gradient to the deformation of the lattice vectors [26]. Thus the lattice view of the material at the phase boundary correlates with the continuum description.

For simplicity, in this work we choose $\alpha = 1-\delta$ and $\gamma = 1+\delta$. For $\delta \ll 1$, the condition that $\det \boldsymbol{U}_1 = 1$ is also approximately satisfied. Under this condition, it can be easily seen that $\hat{\boldsymbol{b}} = \boldsymbol{e}_1$ and $\hat{\boldsymbol{m}} = \boldsymbol{e}_2$. Also the angle of rotation of the martensite variant about the x_3 axis for compatibility with the austenite phase is given by $\theta \approx 0$.

A schematic of the reference configuration of the stress-free austenite phase is shown in Fig. 1(a). A phase boundary between the austenite phase and a martensite variant $\mathcal{P}$ is shown in Fig. 1(b). Figure 1(c) shows a schematic of the lattice underlying the continuum description.

2.2. Energy

The free energy *per unit volume* of a thermoelastic material in a continuum description is taken to be a function of the deformation gradient tensor $\boldsymbol{F}$ and temperature θ. As a consequence of material frame-indifference, the free energy is considered of the form

$$\psi = \tilde{\psi}(\boldsymbol{E}, \theta), \tag{4}$$

where $\boldsymbol{E} = \frac{1}{2}\left(\boldsymbol{F}^T\boldsymbol{F} - \mathbf{I}\right)$ is the Lagrangian or Green strain tensor.

The Lagrangian strain tensor for our choice of transformation stretches can be calculated to be

$$\boldsymbol{E}_1 = \begin{pmatrix} \frac{\alpha^2+\gamma^2}{2} - 1 & \frac{\alpha^2-\gamma^2}{2} & 0 \\ \frac{\alpha^2-\gamma^2}{2} & \frac{\alpha^2+\gamma^2}{2} - 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \delta^2 & 2\delta & 0 \\ 2\delta & \delta^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{5}$$

For a material undergoing phase transformations, the free energy is a non-convex free function of the Lagrangian strain tensor $\boldsymbol{E}$ and temperature θ, $\psi = \hat{\psi}(\boldsymbol{E}, \theta)$. Specifically it is taken to possess multiple minima: a single minimum corresponding to the austenite phase above a transformation temperature θ_T and minima corresponding to the variants of martensite below the transformation temperature. To be precise,

$$\begin{aligned} &\hat{\psi}(\boldsymbol{E}, \theta) > \hat{\psi}(\mathbf{0}, \theta) \text{ for } \theta > \theta_T,\ \forall \boldsymbol{E} \neq \mathbf{0} \\ &\hat{\psi}(\boldsymbol{E}, \theta_T) > \hat{\psi}(\mathbf{0}, \theta_T) = \hat{\psi}(\boldsymbol{E}_i, \theta_T) \text{ for } \forall \boldsymbol{E} \neq \mathbf{0}, \boldsymbol{E}_i, i = 1, 2, \ldots, 6, \\ &\hat{\psi}(\boldsymbol{E}, \theta) > \hat{\psi}(\boldsymbol{E}_i, \theta) \text{ for } \theta < \theta_T,\ \forall \boldsymbol{E} \neq \boldsymbol{E}_i, i = 1, 2, \ldots, 6. \end{aligned} \tag{6}$$

A free energy function possessing these properties can be systematically constructed using the symmetry strain invariants of the parent phase in the form of a Landau polynomial expansion as given in [27].

The strain components describing the martensite well can be seen to satisfy $E_{11}+E_{22} = 2\delta^2$, and $E_{12} = 2\delta$ from Eq. (5). The energy can be a taken to be a function of the normalized invariants [27]

$$I_1 = \frac{E_{11}+E_{22}}{2\delta^2}, \quad I_2 = \frac{E_{11}E_{22}}{4\delta^4}, \quad I_5 = \frac{E_{12}^2}{\delta^2}. \tag{7}$$

We construct a free energy function of the form

$$\psi(I_1, I_2, I_5, \theta) = d_1(I_1^2 - I_2) + d_2 I_1^2 \left[\left(I_1 - \frac{3 - \sqrt{1 - 4h(\theta)}}{2}\right)^2 + h(\theta)\right] + d_3\left(-I_1 I_5 + \frac{I_5^2}{2}\right), \tag{8}$$

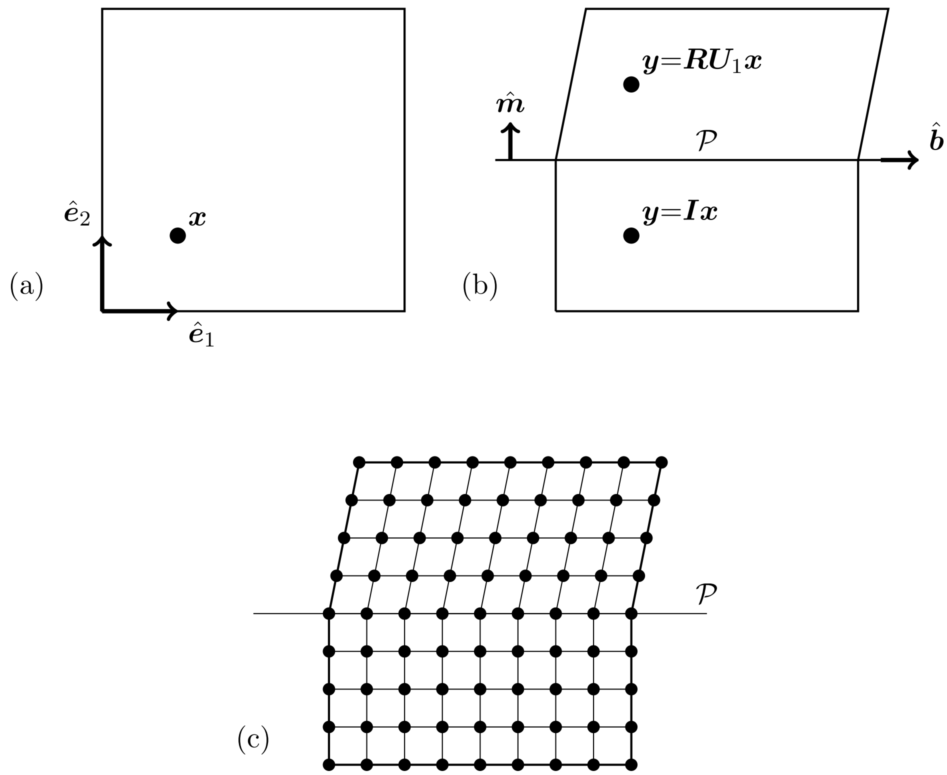


Figure 1: (a) Reference austenite configuration. (b) Partially transformed martensite. The phase boundary $\mathcal{P}$ has a normal $\hat{\boldsymbol{m}}$. (c) The underlying lattice in the deformed configuration.

where d_1, d_2, d_3 are positive constants and $h(\theta) \leq 0.25$ gives the energy difference between the martensite and austenite wells and is a monotonically increasing function of temperature θ. Further, at the transformation temperature $h(\theta_T) = 0$.

3. Frenkel-Kontorova model

The Frenkel-Kontorova model was originally proposed in the context of an edge dislocation propagating through a lattice. It has been later extended to study screw dislocations, cracks, twin and phase boundaries. The main simplifications of the model are to consider the entire dislocation line as a single degree of freedom and study the dynamics of the rows of atoms on the plane in which the dislocation line propagates. The masses of all the atoms are also considered to be uniform in this simple model. In this section we describe this model in the context of a phase boundary.

Figure 2 shows a schematic view of the underlying lattice as a phase boundary propagates through the material. Under an applied resolved shear stress τ, propagation of the boundary from its initial location $\mathcal{P}_0$ to its current location $\mathcal{P}_1$ occurs through the motion of a ledge *along* the phase boundary [28, 29]. A schematic view of this ledge is shown in Fig. 2(c). In the Frenkel-Kontorova model, the atoms on $\mathcal{P}_t$ are considered. To the left of the gray shaded ledge, $\mathcal{P}_t$ is the phase boundary whereas to the right of the ledge the material is transformed into the martensite phase on $\mathcal{P}_t$.

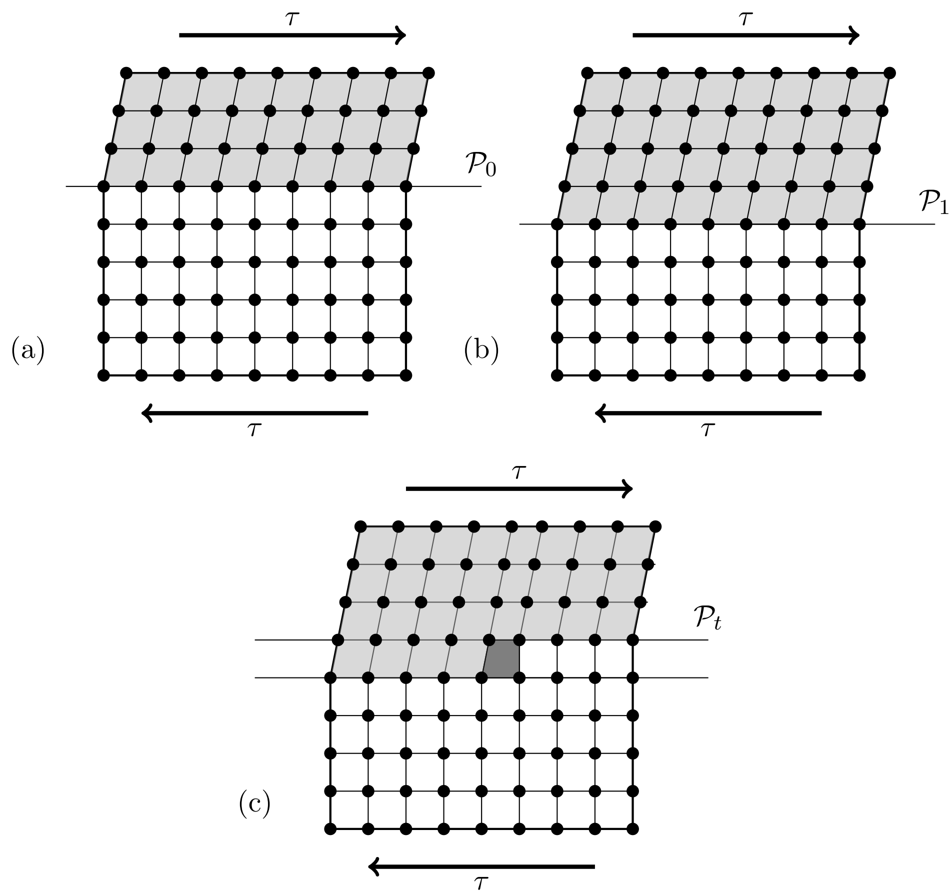


Figure 2: (a) The lattice showing the location of the phase boundary $\mathcal{P}_0$. (b) Phase boundary $\mathcal{P}_1$ after motion by one lattice spacing. (c) Schematic of a ledge on the phase boundary. The ledge is shaded dark gray. The propagation of the ledge to the right results in a downward propagation of the phase boundary.

3.1. Governing equations

We consider the dynamics of the nth particle on the plane $\mathcal{P}_t$. The equation of motion of the nth particle is

$$m\ddot{u}_n = -\Phi'(u_n) + f, \tag{9}$$

where m is the mass of each particle and f represents the applied resolved shear stress on the phase boundary. $\Phi(u_n)$ is the total interaction energy of particle n with all its neighbors.

The key idea of the Frenkel-Kontorova formulation is to consider the interaction to be composed of harmonic nearest neighbor interactions along the phase boundary and anharmonic interactions with the rest of the surrounding atoms. Thus Φ is taken to be of the form

$$\Phi(u_n) = \frac{1}{2}s(u_{n+1} - u_n)^2 + \frac{1}{2}s(u_n - u_{n-1})^2 + \bar{W}(u_n), \tag{10}$$

where s is the stiffness.

The energy $\bar{W}(u_n)$ arises due to a change in the atomic position on ledge from the parent austenite configuration to the martensite phase. As discussed earlier, the kinetics of this transformation is a simple shear. Thus the energy change associated with this process can be obtained

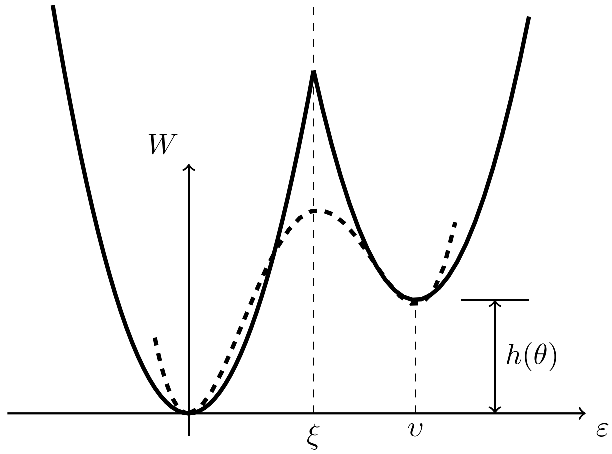


Figure 3: Energy per atom of the lattice as a function of the shear of the lattice ε. The free energy presented in Eq. (8) is shown as a function of the parameter ε as a dashed line. The solid lines represent a piecewise parabolic approximation.

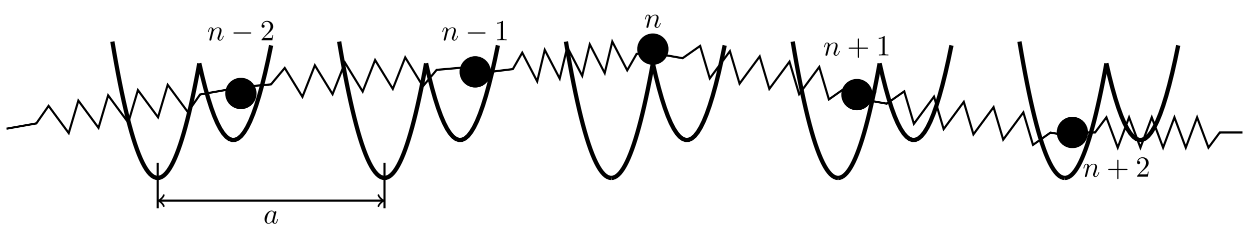


Figure 4: Frenkel-Kontorova model of the atoms on the phase boundary plane $\mathcal{P}_t$. Each particle experiences a substrate potential given by Eq. (11). The distance between the periodic wells is the lattice spacing of austenite a.

from Eq. (8) by parametrizing through the shear ε. The parametrized equation is shown in Fig. 3 using a dashed line. In this work, we approximate $W(\varepsilon)$ as two piecewise parabolas shown with solid lines in Fig. 3. The specific form of $\hat{W}$ is chosen to be

$$\hat{W}(\varepsilon,\theta) = \begin{cases} \frac{1}{2}\mu\varepsilon^2, & \varepsilon \leq \xi(\theta), \\ \frac{1}{2}\mu(\varepsilon - \varepsilon_m)^2 + h(\theta), & \varepsilon \geq \xi(\theta), \end{cases} \tag{11}$$

where μ is the shear modulus. The parameter $\xi(\theta)$ represents the intersection of the two energy wells and is given by

$$\xi(\theta) = \frac{\upsilon}{2} + \frac{h(\theta)}{2\mu\upsilon}. \tag{12}$$

Since we consider only the position of the atom on the phase boundary and the motion is in the direction of shear, the energy per atom due to all the neighboring particles not on the phase boundary can be taken as a function of the atomic position u_n and is thus $\hat{W}(u_n,\theta)$. Thus the temperature θ changes the energy per unit atom and thus influences its dynamics.

With this specific form of the interaction energy, the equation of motion for the nth particle becomes

$$m\ddot{u}_n = s\left(u_{n+1} - 2u_n + u_{n-1}\right) + f - \frac{\partial \hat{W}(u_n,\theta)}{\partial u_n}. \tag{13}$$

3.2. Quasicontinuum approximation

In order to obtain information at macroscopic length scales, it is interesting to study the continuum limit of the Frenkel-Kontorova model. There have been several different different approaches to obtain such continuum limits. A polynomial based Boussinesq was used by Abeyaratne and Vedantam [7] to obtain a quasicontinuum approximation. However, the strain gradient part of the elastic energy in this model is not positive definite [30]. Thus the initial-value problem for the Boussinesq model is linearly ill-posed and has unbounded growth rates at short wavelengths [31, 32].

Alternatively a rational approximation of the difference term has been considered with the advantage of always being stable at short wave lengths [33].

A detailed study of these two approaches has shown that both the models present qualitatively similar kinetic relations which are comparable to the discrete kinetic relation [34]. For this reason, we only consider the polynomial approximation of the difference term in this paper [7]. In the continuum limit, the particle displacement $u_n(t)$ is replaced by a continuous displacement $u(x,t)$ chosen such that $u_n = u(na,t)$ where a is the interparticle spacing in the reference configuration.

Then the equations of motion Eq. (13) in terms of the continuous displacement field take the form

$$m\frac{\partial^2 u}{\partial t^2} = s\left(u(x+a,t) - 2u(x,t) + u(x-a,t)\right) + f - \begin{cases} \mu u, & u < \xi(\theta), \\ \mu(u-\upsilon), & u > \xi(\theta). \end{cases} \tag{14}$$

The quasicontinuum approximation of the governing equation is obtained by replacing $u(x \pm a, t)$ in Eq. (13) by five terms (see [7]) of the series expansion to obtain

$$m\frac{\partial^2 u}{\partial t^2} = sa^2\frac{\partial^2 u}{\partial x^2} + \frac{sa^4}{12}\frac{\partial^4 u}{\partial x^4} + f - \begin{cases} \mu u, & u < \xi(\theta), \\ \mu(u-\upsilon), & u > \xi(\theta). \end{cases} \tag{15}$$

4. Results

We first explore steady traveling wave solutions of the problem. Such motions arise when the ledge propagates at a constant speed. If the motion propagates from one atom to the next at a steady speed, say c, then the motion of the $(n+p)$th atom is identical to that of the nth atom but with a time delay pa/c. For such a motion

$$u_{n+p}(t) = u_n\left(t - \frac{pa}{c}\right). \tag{16}$$

Such a steady motion can occur if and only if $u_n(t)$ has the traveling wave form

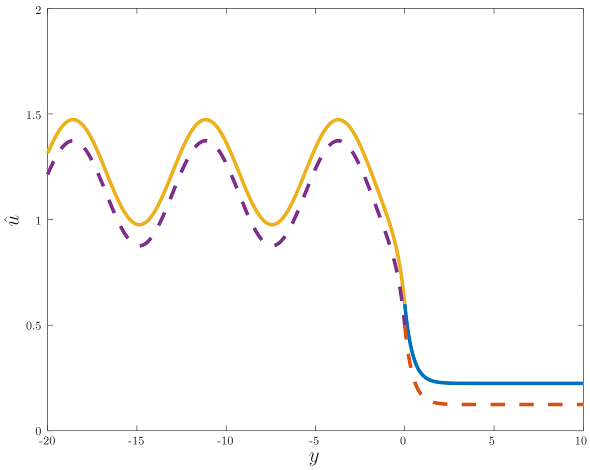
$$u_n(t) = u(na - ct). \tag{17}$$

In terms of the continuum displacement $u(x,t)$ the traveling wave form that we seek is of the form

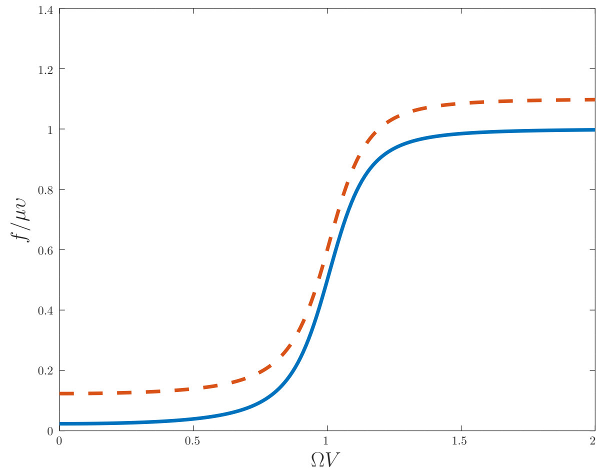
$$u(x,t) = \hat{u}(y), \quad y = x - ct. \tag{18}$$

In the traveling wave form, Eq. (15) becomes

$$\frac{sa^4}{12}\hat{u}'''' + (sa^2 - mc^2)\hat{u}'' + f = \begin{cases} \mu\hat{u}, & \hat{u} < \xi(\theta), \\ \mu(\hat{u}-\upsilon), & \hat{u} > \xi(\theta). \end{cases} \tag{19}$$



(a)



(b)

Figure 5: (a) Solution of the quasicontinuum problem for two different values of the non-dimensional temperature. Solid line is for $\bar{\theta} = 0$ and dashed line is for $\bar{\theta} = 0.1$. (b) Kinetic relations for the corresponding temperatures.

We consider a single ledge propagating along the phase boundary to the right such that the austenite phase is transformed to martensite as shown in Fig. 2(c). In such a case, taking the ledge to be at the origin of the traveling wave coordinate, the boundary conditions are

$$\begin{aligned} \hat{u} &< \xi, \quad y \to \infty, \\ \hat{u} &> \xi, \quad y \to -\infty. \end{aligned} \tag{20}$$

Equation (19) can then be rewritten under these conditions as

$$\frac{sa^4}{12}\hat{u}'''' + (sa^2 - mc^2)\hat{u}'' + f = \begin{cases} \mu\hat{u}, & y > 0, \\ \mu(\hat{u} - \upsilon), & y \le 0. \end{cases} \tag{21}$$

Since we have chosen the origin of the traveling wave coordinate $y = 0$ at the intersection of the austenite and martensite wells, we impose the following conditions

$$\hat{u}'(0+) = \hat{u}'(0-) = \xi(\theta). \tag{22}$$

Additionally, we require the first three derivatives to be continuous at $y = 0$. Under these conditions and the boundary conditions given in Eqs. (20), the solution of Eq. (21) is given by

$$\hat{u}(y) = \begin{cases} \frac{f}{\mu} + \left(\frac{\upsilon}{2} + \frac{h(\theta)}{2\mu\upsilon} - \frac{f}{\mu}\right)\exp\left(-w_1 y\right), & y \ge 0, \\ \upsilon + \frac{f}{\mu} - \left(\frac{\upsilon}{2} + \frac{h(\theta)}{2\mu\upsilon} - \frac{f}{\mu}\right)\exp\left(w_1 y\right) + 2\left(\frac{h(\theta)}{2\mu\upsilon} - \frac{f}{\mu}\right)\cos\left(w_2 y\right), & y \le 0, \end{cases} \tag{23}$$

along with the kinetic relation

$$\frac{f}{\mu\upsilon} = \left\{\frac{h(\theta)}{2\mu\upsilon^2} + \frac{1}{2}\left[1 - \frac{1 - \Omega^2 V^2}{\sqrt{(1 - \Omega^2 V^2)^2 + \mu/(3s)}}\right]\right\}, \tag{24}$$

where

$$
\begin{aligned}
w_1 &= \sqrt{6}\left\{\sqrt{(1-\Omega^2V^2)^2+\mu/(3s)}+(1-\Omega^2V^2)\right\}^{1/2} > 0, \\
w_2 &= \sqrt{6}\left\{\sqrt{(1-\Omega^2V^2)^2+\mu/(3s)}-(1-\Omega^2V^2)\right\}^{1/2} > 0
\end{aligned} \tag{25}
$$

and we have set the non-dimensional velocity $\Omega^2V^2 = mc^2/sa^2$.

The solution to the quasicontinuum problem given by Eq. (23) and the kinetic relation Eq. (24) are plotted in Fig. 5(a) and Fig. 5(b) respectively, taking the parameters $h(\theta)/2\mu v^2 = \bar{\theta}$ where $\bar{\theta} = \theta/\theta_T$ is a non-dimensional temperature. Equation (24) indicates that the driving force required to propagate the phase boundary at a given velocity increases with temperature. The kinetic relation shows a classical form with a critical driving force below which the ledge does not propagate. The value of the critical driving force increases with temperature.

As the ledge propagates to the right, waves are emanated from the ledge behind it (Fig. 5(a)). The effect of the temperature is to increase the resistance to the propagation. The amplitude of the waves is independent of the temperature but the mean particle positions ahead as well as behind the ledge increase with temperature.

5. Conclusions

We have derived a Frenkel-Kontorova model of an austenite-martensite phase boundary between a cubic austenite phase and an orthorhombic martensite phase. Under certain conditions of the transformation stretches between the two phases, the phase boundary connects the two phases through a simple shear deformation. Based on a Landau polynomial expansion of the free energy in terms of the invariants of the Lagrangian strain for such a material, we obtain a substrate potential for particles on the phase boundary. Assuming that the phase boundary propagates by means of a propagating ledge, as observed in experiments, the equations governing the Frenkel-Kontorova model are derived. A quasicontinuum approximation of the FK equations is also studied in order to obtain an analytical description of the phase boundary motion. The solution of the traveling wave problem for the quasicontinuum model indicates that a critical driving force is required in order to drive the ledge and the driving force for ledge propagation increases with temperature.

References

[1] J. N. Reddy, An Introduction to Continuum Mechanics, Cambridge University Press (2013).

[2] J. N. Reddy, An Introduction to Nonlinear Finite Element Analysis: with applications to heat transfer, fluid mechanics, and solid mechanics , Oxford University Press (1985).

[3] R. Phillips, Crystals, Defects and Microstructures Modeling Across Scales, Cambridge University Press (2001).

[4] R. Abeyaratne, J. K. Knowles, On the driving traction acting on a surface of strain discontinuity in a continuum, J. Mech. Phys. Solids 38 (3) (1990) 345–360. doi:10.1016/0022-5096(90)90003-M.

[5] R. Abeyaratne, J.K. Knowles, Kinetic relations and the propagation of phase boundaries in solids, Arch. Ration. Mech. Anal. 114 (1991) 119–154.

[6] R. Abeyaratne, J. Knowles, On the kinetics of an austenite–martensite phase transformation induced by impact in a CuAlNi shape-memory alloy, Acta Mater. **45**, 1671 (1997).

[7] R. Abeyaratne, S. Vedantam, A lattice-based model of the kinetics of twin boundary motion, J. Mech. Phys. Solids 51 (9) (2003) 1675–1700. doi:10.1016/S0022-5096(03)00069-3.

[8] K. Tůma, S. Stupkiewicz, H. Petryk, Size effects in martensitic microstructures: Finite-strain phase field model versus sharp-interface approach, J. Mech. Phys. Solids 95 (2016) 284–307. doi:10.1016/j.jmps.2016.04.013.

[9] R. Ahluwalia, S. S. Quek, D. T. Wu, Simulation of grain size effects in nanocrystalline shape memory alloys, J. Appl. Phys. 117 (2015) 244305. doi:10.1063/1.4923044.

[10] S. Vedantam, Constitutive equations for rate-dependent pseudoelastic behaviour of shape memory alloys, Smart Mater. Struct. **15** (2006) 1172.

[11] F. Hildebrand, R. Abeyaratne, An atomistic investigation of the kinetics of detwinning, J. Mech. Phys. Solids, **56** (2008) 1296.

[12] E. B. Tadmor, M. Ortiz, R. Phillips, Quasicontinuum analysis of defects in solids, Phil. Mag. A, 73 (1996) 1529-1563.

[13] P. M. Gullett, M. F. Horstemeyer, M. I. Baskes, H. Fang, A deformation gradient tensor and strain tensors for atomistic simulations, Model. Simul. Mater. Sci. Eng. 16 (1) (2008) 015001. doi:10.1088/0965-0393/16/1/015001.

[14] J. A. Zimmerman, D. J. Bammann, H. Gao, Deformation gradients for continuum mechanical analysis of atomistic simulations, Int. J. Solids Struct. 46 (2) (2009) 238–253. doi:10.1016/j.ijsolstr.2008.08.036.

[15] G. Wang, A. Al-Ostaz, A. H. D. Cheng, P. R. Mantena, Hybrid lattice particle modeling: Theoretical considerations for a 2D elastic spring network for dynamic fracture simulations, Comput. Mater. Sci. 44 (4) (2009) 1126–1134. doi:10.1016/j.commatsci.2008.07.032.

[16] G. Puglisi, L. Truskinovsky, Mechanics of a discrete chain with bi-stable elements, J. Mech. Phys. Solids 48 (1) (2000) 1–27. doi:10.1016/S0022-5096(99)00006-X.

[17] J. Frenkel, T. Kontorova, On the theory of plastic deformation and twinning. Proc. Z Sowj. 13 (1938) 1–10.

[18] E. Fermi, J. Pasta, S. Ulam, Studies of Nonlinear Problems, Techical Report LA-1940, Los Alamos Scientific Laboratory (1955).

[19] W. Atkinson, N. Cabrera, Motion of a Frenkel-Kontorowa dislocation in a one-dimensional crystal, Phys. Rev. 138 (3A) (1965) 763–766. doi:10.1103/PhysRev.138.A763.

[20] S. Vedantam, S. Mohanraj, Structural phase transitions in a discrete one-dimensional chain, Int. J. Appl. Mech. 01 (03) (2009) 545–556. doi:10.1142/S1758825109000290.

[21] L. Truskinovsky, A. Vainchtein, Solitary waves in a nonintegrable Fermi-Pasta-Ulam chain, Phys. Rev. E 90 (2014) 042903.

[22] L. Truskinovsky, A. Vainchtein, Kinetics of martensitic phase transitions: Lattice model, SIAM J. Appl. Math. 66 (2) (2006) 533–553. doi:10.1137/040616942.

[23] U. Mahendaran, B. C. Rao, S. Vedantam, Constitutively informed multi-body interactions for lattice particle models, Comp. Meth. Appl. Mech Engg., (2020) *in press*.

[24] K. F. Hane, T. W. Shield, Microstructure in a Cubic to Orthorhombic Transition, J. Elas. 59 (2000) 267-318.

[25] M. Charlotte, L. Truskinovsky, Lattice dynamics from a continuum viewpoint, J. Mech. Phys. Solids 60 (8) (2012) 1508–1544. doi:10.1016/j.jmps.2012.03.004.

[26] J. L. Ericksen, On the Cauchy-Born rule, Math. Mech. Solids 13 (3-4) (2008) 199–220. doi:10.1177/1081286507086898.

[27] S. Vedantam, R. Abeyaratne, A Helmholtz free-energy function for a Cu-Al-Ni shape memory alloy, Int. J. Non. Linear. Mech. 40 (2-3) (2005) 177–193. doi:10.1016/j.ijnonlinmec.2004.05.005.

[28] J. P. Hirth, R.C.Pond, Steps, dislocations and disconnections as interface defects relating to structure and phase transformations, Acta Mater., 44, (1996) 4749–4763.

[29] D. Bray, J. Howe, High-resolution transmission electron microscopy investigation of the face-centered cubic/hexagonal close-packed martensite transformation in Co-31.8 wt pct Ni alloy: Part 1. Plate interfaces and growth ledges, Metall. Mater. Trans. A **27A**, (1996) 3362-3370.

[30] I. A. Kunin, Elastic Media with Microstructure. 1. One-dimensional Models. Springer, New York. (1982).

[31] R.L. Pego, P. Smereka, M.I. Weinstein, Oscillatory instability of solitary waves in a continuum model of lattice vibrations. Nonlinearity 8 (1995) 921–941.

[32] C. I. Christov, G. A. Maugin, M. E. Velarde, Well-posed Boussinesq paradigm with purely spatial higher-order derivatives. Phys. Rev. E 54 (1996) 3621–3638.

[33] P. Rosenau, Dynamics of nonlinear mass spring chains near the continuum limit. Phys. Rev. Lett. A 118 (5) (1986) 222–227.

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