A Comprehensive Dynamical Study of Nucleation and Growth in a One–Dimensional Shear Martensitic Transition

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Abstract

We have constructed a complete hydrodynamic theory of nucleation and growth in a one–dimensional version of an elastic shear martensitic transformation with open boundary conditions where we have accounted for interfacial energies with strain–gradient contributions. We have studied the critical martensitic nuclei for this problem: Interestingly, the bulk critical nuclei are twinned structures, although we have determined that the dominant route for the formation of martensite is through surface nucleation. We have analytically solved for the surface nuclei and evaluated exact nucleation rates showing the strong preference for surface nucleation. We have also examined the growth of martensite: There are two possible martensitic growth fronts, viz., dynamical twinning and so-called two–kink solutions. These transformation fronts are separated by a dynamical phase transition. We analytically derive this phase diagram and determine expressions for the speeds of the martensitic growth fronts.
1. INTRODUCTION AND MOTIVATION:

Nature offers a variety of transformations between different crystallographic states. For many crystals, the result of such a phase transition involves a dramatic change in the macroscopic shape of the material. Quite often, associated with these macroscopic changes is the formation of characteristic domain patterns, sometimes called microstructure. When viewed under a transmission electron microscope (TEM), the most commonly observed microstructures are those related to twinning, \textit{viz.}, symmetry related variants of the product phase(s) oriented in a characteristic pattern. The study of these materials is very desirable because many technologically important compounds, such as shape memory alloys and the A15 superconductors, undergo what are commonly known as martensitic transformations — these transformations lead to the formation of the microstructure discussed above.

Martensites are to be distinguished from other materials undergoing structural phase transitions by the non–diffusive nature of the transition. To be specific, (i) if the structural transformation occurs without a net diffusion of atoms across the crystalline unit cell boundary, (ii) the transition is discontinuous (also referred to as first–order), and (iii) the transformation involves shear strains, the transformation is said to be martensitic, and the resulting material a martensite. These transformations can always be described in terms of strains and possibly lattice modulations (or so-called lattice vibrational modes). Here we shall specialize to a subclass of martensitic transitions known as proper ferroelastic transitions for which the only relevant variables are the purely elastic strains.

Martensitic transformations occur by a nucleation and growth processes, and the dynamical path by which such transformations proceed is the subject of this paper. We explore the dynamical evolution of a phenomenological model of a one–dimensional, purely elastic, martensitic transformation based on the concept of a strain order parameter. We determine both the nucleation and dynamical growth aspects of the transformation for this simple model. We also make contact with the formation of microstructure, something that Bales and one of us has recently proposed can be associated with the dynamics of martensitic
The consideration of a lower dimensional model has many advantages: Firstly, many of the practical problems (e.g., numerical integration of the equation of motion) associated with higher dimensional systems are eliminated. Secondly, lower dimensional systems often allow for the possibility of obtaining exact analytical results. We shall indeed find many exact analytical solutions, and hopefully these results will be able to be extended into higher dimensions in the future.

Summarizing our main findings:

I – One may numerically solve for the bulk critical nucleus for such transformations, and then obtain an excellent analytical approximation to this structure. The bulk critical nucleus is twinned.

II – For any finite system with open boundary conditions, the critical nucleus may be solved for exactly, and we find that it exists at the surface of the system. It’s energy is (almost exactly) four times less than that of the bulk nucleus (namely, the critical nucleus for a system of infinite extent), and it is not twinned.

III – As shown previously [4], interesting domain wall motions are associated with the growth of martensite when the system is quenched to temperature below the transition temperature. Here we will show that one can understand the variety of growth fronts that are found for these dynamics by analytically deriving interfacial growth speeds for a variety of domain walls, and then applying a local stability analysis.

We believe that apart from the inclusion of thermal fluctuations, something that would require simulations based on, e.g., Langevin dynamics, this work represents as complete a numerical plus analytical examination of this one–dimensional problem as is possible.

Our paper is organized as follows. In Section 2 we provide all of the requisite mathematical formalism to understand our one–dimensional model system. Then, in Section 3 we determine the critical nucleus for both bulk and surface nucleation, with particular attention paid to the intimate relation between the bulk and surface solutions. Section 4
provides a comprehensive study of the growth dynamics that can occur for initial states that are supercritical. We also provide analytical work that successfully explains much of the observed numerical results, and allows for the exact derivation of various dynamically interesting quantities (i.e., the growth speed of a transformation front). We have tried to compare, wherever possible, our numerical results to those of relevant experiments. Lastly, in Section 5 we summarize our results, and forecast the success of similar phenomenologies to the more interesting case of higher dimensional systems.

2. FORMALISM AND THE EQUATION OF MOTION:

In this section we will present the formalism necessary to describe a model of a one-dimensional (1D) version of a first-order, elastic shear transformation via a Ginzburg–Landau (GL) theory. This model was first applied to martensite by Falk [3], and we believe that it is the simplest GL potential depending on only one spatial variable that includes any of the important characteristics of these transitions. For example, we wish to focus on martensitic transitions wherein the high-temperature parent phase has a sufficiently high symmetry that the transformation shear strains lead to degenerate martensitic product states, something that is a prerequisite for the formation of twinning — we use Falk’s GL potential since it possesses this feature.

Falk’s mean-field theory of martensitic phase transitions lies in the construction of the phenomenological GL free-energy density. To be specific, one considers a displacement field \( u(x,t) \) and the associated strain \( e(x,t) = \partial u/\partial x \equiv \partial_x u \). Then, one imagines that the local free energy density, \( f_L \), of the system can be characterized by a nonlinear function of the form:

\[
f_L(e) = \frac{1}{2} A \delta T e^2 - \frac{1}{4} B e^4 + \frac{1}{6} C e^6 .
\]

(1)

In Eq. (1), \( A, B, \) and \( C \) are positive, temperature independent, phenomenological constants and \( \delta T = T - T_c \). The quantity \( T_c \) represents the temperature at which the unstrained
parent phase \((e = 0)\) becomes unstable. In a linear theory, the undercooling, \(\delta T\), would be related to the linear elastic constant \(c\) of the high-temperature parent phase by \(c = A \delta T\).

The first three terms in the Landau energy density above represent the local response of the system to a given strain. The particular symmetry of the local potential, \(viz.\ f_L(e) = f_L(-e)\), ensures that both positive and negative shear strains of equal magnitude have the same energy. For an appropriate choice of model parameters, a local free energy density similar to the one illustrated in Fig. 1 can be produced. GL densities of this form can be attributed to systems for which the (high-temperature) parent phase and (low-temperature) product phase(s) are separated by a first-order, elastic shear transformation.

In our model, temperatures greater than the first-order transition temperature, \(T_1\), lead to only one absolute minimum, \(e = 0\), on the energy surface; this strain state corresponds to the parent phase. Below \(T_1\), the parent state becomes metastable and two doubly degenerate, stable minima develop at \(e = \pm e_m\) (the so-called martensitic strains). These minima correspond to symmetry related variants of the product phase and are often referred to as martensitic twins.

We also wish to include so-called non-local elastic forces. For the one-dimensional problem that we are considering, the appropriate form of this energy is

\[ f_{NL} = \frac{1}{2} D(\partial_x e)^2 \quad . \]

Terms of this form are responsible for many properties. Firstly, they account for non-local forces associated with inhomogeneous strain fields. Secondly, in the context of phase-transition theory, such terms represent the domain-wall energy associated with the inhomogeneities of two-phase regions (this is the analogue of the so-called Ginzburg energy found in the theory of type-II superconductors). Lastly, these terms break the scale invariance implicit in Eq. (1) for a bulk system — we shall elaborate on this last feature below.

The total elastic free energy density is thus \(f_L + f_{NL}\), implying that for a system of length \(L\) defined by the spatial range \(-\frac{L}{2} \leq x \leq \frac{L}{2}\) the total elastic free energy is

\[ F = \int_{-\frac{L}{2}}^{\frac{L}{2}} \left[ f_L(x) + f_{NL}(x) \right] dx \quad . \]
In order for the equation of motion to be specified for this system, one could make use of the time–dependent Ginzburg–Landau theory (TDGLT) to construct a first–order in time, nonlinear, nonlocal partial differential equation (PDE) for the dynamical evolution of the system \[6\]. This approach, however, has been shown to lead to a completely incorrect description of the dynamical growth aspects of elastic–shear transformations \[4\]. Instead, one must properly account for the hydrodynamic character of the sound waves through the inclusion of the kinetic energy density associated with the propagating growth interfaces. This approach makes use of the fact that nonlinear elastic models of the type discussed here can be treated as nonconvective, hydrodynamic systems \[7\].

Propagating disturbances in a solid, e.g., thermal phonons, necessarily involve the displacement of a finite mass of material and hence contribute to the total mechanical energy of the system. Recalling that the displacement field, \(u(x,t)\), describes the physical displacements of the atoms in a solid relative to some chosen undistorted system, the kinetic energy, \(T\), is given by

\[
T = \frac{1}{2} \rho \int_{-L}^{L} \left[ \left( \partial_t u \right)^2 \right] dx ,
\]

where \(\rho\) is the linear mass density of the undistorted bar. In the spirit of our hydrodynamic considerations, we also include a Rayleigh dissipation function, \(R\), with sound wave viscosity \(\gamma\), viz.,

\[
R = \frac{1}{2} \gamma \int_{-L}^{L} \left[ \left( \partial_t \partial_x u \right)^2 \right] dx ,
\]

that allows for the dissipation of energy of the sound waves \[8\]. It is to be stressed that accounting for the damping in this manner ensures that the sound waves are always propagating at sufficiently long wavelengths; this is the sense in which the system’s hydrodynamic character is being properly accounted for \[9\].

With these ingredients, the equation of motion plus the boundary conditions may be determined precisely as described, e.g., in Ref. \[7\] — we stress that we are studying a finite system, and thus the boundary conditions are an important part of this problem. The bulk equation of motion for the system is
\[ \rho(\partial_t^2 u) = \rho \partial_x^2 \left[ A \delta T - 3B \partial_x u \right]^2 + 5C(\partial_x u)^4 \right] - D(\partial_x^4 u) + \gamma (\partial_t \partial_x^2 u) \right], \tag{6} \]

and the four boundary conditions are

\[ A \delta T \partial_x u - B(\partial_x u)^3 + C(\partial_x u)^5 + \gamma (\partial_x \partial_t u) - D(\partial_x^3 u) = 0 \text{ at } x = \pm \frac{L}{2} \tag{7} \]

and

\[ (\partial_x^2 u) = 0 \text{ at } x = \pm \frac{L}{2} \tag{8} \]

By differentiating Eq. (6) once, these equations can also be conveniently restated in terms of the shear strain:

\[ \rho(\partial_t^2 e) = \partial_x^2 \left[ A \delta T e - Be^3 + C e^5 - D(\partial_x^2 e) + \gamma (\partial_t e) \right] \right], \tag{9} \]

with boundary conditions

\[ (\partial_t e) = \frac{1}{\gamma} \left( D(\partial_x^2 e) - A \delta T e + Be^3 - C e^5 \right) \tag{10} \]

and

\[ (\partial_x e) = 0, \text{ at } x = \pm \frac{L}{2} \tag{11} \]

In certain instances (see below) it will be advantageous to refer to the constitutive equations in this form.

These equations involve a large number (eight) of material parameters. However, we can substantially reduce the number of parameters required to model our system through scaling analysis, and the result of this analysis for bulk systems has been discussed elsewhere \[4,17\]. Here we are considering systems of a finite length, and have chosen to rescale our dynamical equations through the use of a generalized dimensional analysis for boundary valued problems \[10\]. The mathematical details of this are summarized in the Appendix A; the physics behind the resulting equation of motion and boundary conditions are as follows: There are four dynamical units, \textit{viz.}, distance, time, mass and temperature. Rescaling the “length” of each of these four dynamical units allows us to eliminate four of the material
parameters. Further, we can scale the two parameters depending only on lengths, \( x \) and the displacement field \( u \), using different scale factors (this is analogous to simply rescaling the unit strain), and thus we find that we can reduce our problem down to one involving only three material parameters, \( \Lambda \), the scaled mass density, \( \delta T \), the scaled undercooling, and \( \tilde{L} \), the scaled length of the system. The resulting equation of motion and boundary conditions are

\[
\Lambda (\partial_t^2 u) = (\partial_x^2 u)[\delta T - 3(\partial_x u)^2 + 5(\partial_x u)^4] - (\partial_x^4 u) + (\partial_t \partial_x^2 u) ,
\]

(12)

\[
\delta T(\partial_x u) - (\partial_x u)^3 + (\partial_x u)^5 + (\partial_x \partial_t u) - (\partial_x^3 u) = 0, \quad \text{at} \quad x = \pm \frac{L}{2} ,
\]

(13)

\[
(\partial_x^2 u) = 0, \quad \text{at} \quad x = \pm \frac{L}{2} ,
\]

(14)

(where in the above system of equations, and from now on, we drop the tildes).

Further, in terms of the scaled variables the local potential is now given by

\[
f_L(x) = \frac{1}{2} \delta T e^2 - \frac{1}{4} e^4 + \frac{1}{6} e^6
\]

(15)

and thus the martensitic strains are now given by

\[
e_m(\delta T) = \pm \sqrt{\frac{(1 + \sqrt{1 - 4\delta T})}{2}} .
\]

(16)

Thus, one has the following sequence for the relative stability of the unstrained and martensitic states [3]: \( \delta T \geq 1/4 \), only the unstrained state is locally stable; \( 3/16 \leq \delta T \leq 1/4 \), the unstrained state is locally stable and the doubly degenerate martensitic states are metastable; \( 0 \leq \delta T \leq 3/16 \), the unstrained state is metastable and doubly degenerate states are stable; \( \delta T \leq 0 \), only the doubly degenerate martensitic states are locally stable.

### 3. THE CRITICAL NUCLEUS:

In the model discussed above, we have tacitly assumed that the system is coupled to an infinite heat bath so that the dynamics can be considered to be isothermal. However, if the
system is found in the metastable unstrained state at temperatures such that \( \delta T < \frac{3}{16} \), a local fluctuation (of the displacement field) can lead to the subsequent formation of a locally stable region of martensite which can grow to expel (sometimes) all of the unstrained state. That is, the decay of the metastable state (e.g., the unstrained bar) requires an excitation called the “critical nucleus” with finite activation energy \( \Delta E \). Any initial displacement profile that lies “below” this saddle–point configuration will decay to zero, whereas states lying “above” this profile may be able to escape from the basin of attraction and grow to the (globally) stable product phase. In this section we shall describe both the novel twinned nucleus, which characterizes the bulk nucleus of a spatially infinite system, and the localized (in strain) surface states, which correspond to the true critical nuclei (saddle–points) of this problem. Then, in the next section we will provide some examples of the fascinating growth phenomena that can result as the system approaches steady state.

We can find the critical nucleus by solving the following nonlinear ODE plus nonlinear boundary conditions:

\[
\partial_x^4 u - \partial_x^2 u (\delta T - 3 (\partial_x u)^2 + 5 (\partial_x u)^4) = 0 ,
\]

\[
\delta T (\partial_x u) - (\partial_x u)^3 + (\partial_x u)^5 - (\partial_x^3 u) = 0 \quad \text{at} \quad x = \pm \frac{L}{2} ,
\]

\[
(\partial_x^2 u) = 0 \quad \text{at} \quad x = \pm \frac{L}{2} .
\]

The above system of nonlinear equations are derived from considering the static, zero–force case of Eqs. (12,13,14). The bulk or “saddle–point” critical nucleus that we are interested in, to be denoted by \( u_{bcn}(x) \), is the lowest energy, localized configuration satisfying the above set of equations — the localization of the displacement field is a consequence of the physical constraint that for a bulk nucleus, the boundaries must be unaffected by the spatial perturbation. (We stress that this constraint is based on physical considerations, and does not arise from a purely mathematical treatment of the formalism presented in the previous section.)
A. Bulk Solutions:

In this section we consider a system of infinite extent, thus precluding the possibility that the system nucleates at a boundary. For such a bulk critical nucleus, Eqs. (18) and (19) are irrelevant, and the solutions of interest must solve Eq. (12) and satisfy \( \partial_j^nu = 0 \) as \( x \to \pm \infty \) for \( j = 0, \ldots, 4 \).

The work required to find the critical nucleus is greatly simplified by the observation that the equations determining it depend on only one (scaled) material parameter, \( \delta T \).

At this point we choose to refer to the ratio of energies \( \frac{E_W}{E_B} \) instead of \( \delta T \), where \( E_B \) is the energy barrier separating the unstrained state from the martensitic wells, and \( E_W \) is the energy difference between the \( e = 0 \) and \( e = \pm e_m \) wells — these two energies are displayed in Fig. 1. In terms of \( \delta T \)

\[
\frac{E_W}{E_B}(\delta T) = \frac{1 - 6\delta T + (1 - 4\delta T)\sqrt{1 - 4\delta T}}{-1 + 6\delta T + (1 - 4\delta T)\sqrt{1 - 4\delta T}}
\]

and from now on we shall refer to this ratio, quite simply because it better distinguishes between the differing “shapes” of the local Landau potential Eq. (1). Noting that \( \delta T = 1/6 \Rightarrow E_W = E_B \), we have chosen to examine \( \frac{E_W}{E_B} = 0.2, 1.0, \) and \( 5.0 \), corresponding to \( \delta T = 0.1823, 1/6, 0.1295 \).

We an easily determine one feature of the critical bulk nucleus for this system — symmetry arguments plus the physical constraint of a vanishing displacement field at the boundaries allow us to specify that the bulk critical nucleus is a localized, symmetric displacement field. Namely, since localized symmetric states are lower in energy because there are fewer domain walls present, we know that this must be the symmetry of our bulk critical state.

We have solved for the bulk critical nuclei vs. \( \frac{E_W}{E_B} \) numerically. This is a difficult problem since apart from the symmetry of the solution, one does not know \textit{a priori} where in function space to begin one’s search. In order to minimize this difficulty, we have followed an approach based on the full dynamical equations. We assume that the critical nucleus should be a configuration approximately of the form
\[ u(x) = u_0 \exp(-x^2 / d^2) \] \hspace{1cm} (21)

We consider this functional form because it smoothly interpolates between a classical nucleus \((n \to \infty)\) and a Gaussian fluctuation of the displacement field with broad domain walls \((n = 1)\) — these two limiting states are shown in Fig. 2. We then specify that \(d\) is not too narrow, say \(d = 10\) domain wall lengths (see, e.g., Appendix B), and for simplicity take \(n = 1\). Thus, for the static displacement field

\[ u(x) = u_0 \exp(-x^2 / d^2) \] \hspace{1cm} (22)

at \(t = 0\), we numerically integrate forward in time under the dynamics of the system to find the “critical” value of \(u_0\) as a function of \(E_W / E_B\), viz., the value of \(u_0\) for which perturbations above or below will grow or decay respectively. In this way, we have dynamically eliminated those initial configurations which could not possibly be candidates for the critical nucleus.

Having obtained this reduced function space, a numerical solution for the critical nucleus becomes tractable: we employ a numerical relaxation method [11] that solves the zero–force equation (plus boundary conditions) using as input Eq. (22) and the critical value of \(u_0\) found as described above. These bulk critical nuclei for the above–mentioned ratios of \(E_W / E_B\), are shown in Fig. 3. (We stress that these solutions are found for \(L\) being sufficiently large such that if the length of system is then doubled, our solutions are unchanged — this confirms that these are indeed bulk nuclei unaffected by the surfaces.) It is interesting to observe that the critical nucleus is a fully twinned strain state. This may be understood from Fig. 3b where the strain profile for \(E_W / E_B = 1.0\) is displayed. This behaviour is a direct consequence of the physical as opposed to mathematical constraint of a vanishing displacement field at the boundaries, i.e., a localized, twinned strain state allows for the localization of the displacement field. (For example, in any configuration with only one sign of strain throughout the entire system, at least one boundary must be displaced.)

To further check that these numerical solutions behave like saddle–point solutions, we have examined their evolution under the full dynamical equations of motion in two ways:

\[ u_{bcn}(x) \to (1 \pm \epsilon) u_{bcn}(x) \] \hspace{1cm} (23)
where numerically we have used $\epsilon$ values as small as 0.001. In the case of (i), it was found that the $1 - \epsilon$ configuration was always subcritical, while the $1 + \epsilon$ configuration was always supercritical. Further, it was also found that a scaling of the independent variable described in (ii) was supercritical (subcritical) if the state was increased (decreased) in size. Thus, these critical nuclei have just enough driving force (energetically speaking) and are just big enough to drive the system into the martensitic state.

As the ratio $E_W/E_B \to \infty$ (viz., as $\delta T \to 0$), it becomes increasingly difficult to obtain converged saddle-point solutions to the zero-force equations. We find that the critical nucleus becomes more non-classical, viz., more bell-shaped; eventually, it becomes too numerically sensitive to relax to a saddle-point solution. However, in the opposite limit of $E_W/E_B \to 0$, the shape of the critical nucleus approaches that of its classical analogue, viz., the step function found from $n \to \infty$ in Eq. (21), and for this limit we have found that it is possible to produce an excellent approximation to the bulk critical nucleus from purely analytical considerations. The details of this analysis are provided in Appendix B, and here we summarize our results.

We consider the zero-force equations now in terms of the strain variable $e$. Firstly, we focus on the equations for an infinite system with the constraint that $\partial_j e = 0$ at $x = \pm \infty$ and $j = 0, 1, \ldots, 4$. One then finds the solutions

$$e_0(x) = \pm 2\sqrt{6\delta T} \sqrt{\frac{\exp[2\sqrt{\delta T}(x - x_0)]}{3 - 16\delta T + 6 \exp[2\sqrt{\delta T}(x - x_0)] + 3 \exp[4\sqrt{\delta T}(x - x_0)]}}$$

(25)

where $x_0$ is some integration constant. Each of these solutions correspond to a strain field that is symmetric about $x = x_{\text{max}}$ where

$$x_{\text{max}} = x_0 + \frac{1}{4\sqrt{\delta T}} \ln\left(\frac{3 - 16\delta T}{3}\right)$$

(26)

Now note that since $e(x)$ is a symmetric function, we know that the boundaries of the system must be displaced — put another way, the strain field defined in Eq. (25) is not a localized solution. Figure 4 shows a plot of Eq. (25) for $E_W/E_B = 1.0$. A graphical comparison with
the exact localized solutions, *viz.* those found from the relaxation technique [see Fig. 3b], suggest that each of the $\pm e_0(x)$ strain configurations correspond to one half of the strain strain states that make up the twinned bulk critical nucleus. We have tested this conjecture and found that a *linear* combination of the form

$$e(x) = e_0(x - x_0) - e_0(x + x_0)$$

(27)

(which by the even symmetry of Eq. (25) is an odd function, the same symmetry as our numerically determined critical nuclei) does in fact satisfy the bulk zero-force equation *with a small residual error*. This error is a function of $x_0$, a quantity which remains to be determined.

Then, we use this approximation in the following way: if we desire an analytical approximation to our (exact) numerical result, we can find an $x_0$ such that Eq. (27) is as close as possible to the exact strain profile. Thus, define the residual error to be the integral of the square of the difference over the length of the system, and then minimize this quantity with respect to $x_0$. For small $E_W/E_B$, this procedure leads to superb agreement with our (numerically) exact solutions. Figure 5 illustrates the somewhat amazing success of this procedure for $E_W/E_B = 1.0$. At this and lower temperatures we thus find that this function yields an excellent fit to the exact solution shown in Fig. 3b. Since we cannot find analytical solutions for $E_W/E_B \gg 5.0$, this procedure is limited to low values of this ratio.

To understand the success of this approximation, we note that although the nonlinear nature of this problem excludes the possibility of *any* linear combination of zero-force solutions exactly satisfying Eq. (17), such as we have used in Eq. (27), the structures that we are superimposing on one another are like two solitons. The solitons are particle–like entities, and it is usual in soliton theory to ascribe an interaction energy between such particles. Usually [18], this interaction decays as an exponential. Thus, in Eq. (27) we have a soliton interaction energy that goes as $\exp(-2x_0)$. As shown in Fig. 3b, for the ratios of $E_W/E_B$ studied here, the value of $x_0$ is quite large, and thus this interaction is very small. This simple consideration explains the success of our analytical work in producing an approximate
B. A Critical Nucleus at the System’s Surface:

In the previous subsection the bulk critical nuclei were found. We wish to stress that in deriving these configurations the boundary conditions given in Eqs. (18, 19) were effectively ignored due to our consideration of a system of infinite extent. Now we include the boundaries by focusing on a system that is finite in at least one direction. We will show that the bulk critical nuclei are not critical nuclei for these systems — in fact, we shall show and analytically derive that the critical nuclei for systems that include at least one free surface always possess critical nuclei localized at the surface. Such states are found to have a significantly lower energy than the bulk critical nuclei.

We discovered these solutions quite easily — simply note that localized surface states in strain space follow directly from the analytical work on the bulk critical nucleus discussed in Appendix B and explicitly stated in Eq. (25). Indeed, if the localized, single–humped bulk solution \( e_0(x-x_0) \) is centered at one of boundaries, \( x_{\text{max}} = \pm L/2 \), the resulting state satisfies the boundary conditions and provides a stationary solution to the bulk equation, namely Eq. (6). Since such a state is similar to that shown in Fig. 3b and only involves non–zero strains in one fourth of the space that a bulk nucleus exists over, clearly it possesses an energy that is (almost exactly) only one quarter of the energy of the critical nuclei solutions that we found for the bulk.

To see that this is indeed a saddle–point solution for a finite system with free boundaries, we employ a hydrodynamic approach [17]. As in any hydrodynamic theory with a conserved quantity (in this case, momentum), a natural physical interpretation of the equation of motion is that of a continuity equation, viz.,

\[
\partial_t (\Lambda \partial_t u) = \partial_x J ,
\]

(28)

where \( J \), the one dimensional momentum current density of the system, is given by
\[ J = \delta T (\partial_x u) - (\partial_x u)^2 + (\partial_x u)^3 + (\partial_t \partial_x u) - (\partial_x^2 u) \]  \hspace{1cm} (29)

For the case of static, zero–force solutions, the continuity equation dictates that the (one–dimensional) divergence of the momentum current, \( \partial_x J \), must be zero, implying that \( J \) is a constant. For any solution that is localized in space, such as Eq. (25), it trivially follows that in fact \( J = 0 \) (e.g., simply consider a region for which the strain is vanishingly small and thus the constant \( J \) must also vanish). Now note that the nonlinear boundary condition in Eq. (18) is nothing more than the condition that \( J = 0 \) at \( x = \pm L/2 \), and thus this boundary condition is satisfied. The second boundary condition, Eq. (19), is satisfied since we have placed the maximum of the strain bump at the system’s surface.

The natural question that arises is: which of the above–discussed nuclei is the potent nucleus for a large but finite system? To answer this question, recall the common definition of the nucleation rate, \( r \), as the ratio of the probability flux \( j \) across the saddle point to the probability \( n \) to be in the metastable well: \( r = j/n \) (e.g., see the discussion in Ref. [22]).

We can readily provide the nucleation rate \( r \) of a kink at the surface, \( \text{viz.} \),

\[ r = S \exp(-\beta \Delta E/4) \]  \hspace{1cm} (30)

where \( \Delta E \) is the activation energy for the bulk nucleus. (The prefactor \( S \) in front of the Arrhenius term is a rate constant.) The lower activation energy of a nucleus at the boundary compared to that of a bulk nucleus (as mentioned above, this ratio of energies is very nearly exactly 1:4) implies that surface nucleation will always be preferred over homogeneous bulk nucleation, and thus will certainly be the dominant route to the formation of martensite. (Of course, the other common inhomogeneity besides a free surface would be impurities, and these would be expected to compete with the surface for the role of “most potent” nucleation centre.)
4. THE PROPAGATING DYNAMICS OF MARTENSITIC GROWTH FRONTS:

In this section we will describe and examine the dynamical growth aspects of those states which have overcome the nucleation barrier, *viz.*, states that lie “above” the critical nucleus, as they approach their steady state profiles. We will thoroughly explain the observed dependence of the dynamical evolution of the product phase, *viz.*, propagating martensitic growth fronts, on the density \( \Lambda \), the undercooling \( \delta T \) and the length of the system, \( L \) — this complements the brief outline of results for this phenomenon given in Ref. [4]. In these investigations we have numerically obtained the evolution of the system under consideration by using a variant method of lines [14] — this provides a high accuracy integration of the equation of motion, *viz.*, Eq. (6), as well as fully accounting for the time–dependent, nonlinear boundary conditions given in Eqs. (7,8).

To be specific, to investigate the dynamical evolution of martensite, we first specify the parameters characterizing the system, *viz.*, the scaled temperature, length and mass density of the system. (To allow us to focus on a physically relevant range of the scaled mass density parameter, we note that recent experimental work on the purely elastic bcc \( \rightarrow \) fcc transformation of pure Lanthanum [15] motivates an initial choice of the \( \Lambda \) parameter of about one [13]. Also, since we are not interested in the dynamics of unstable systems we restrict our attention to \( 0 < \delta T < \delta T_1 \).) Then, we choose an initial displacement field that is both static and supercritical; *e.g.*, for most of our dynamical studies we used the supercritical state defined in Eq. (23) with \( \epsilon \approx 0.01 \). Finally, we employ our numerical integration algorithm [14] to follow the temporal evolution of our system. We stress that the symmetry and/or profile of the initial state does not qualitatively influence the interfacial dynamics observed, *viz.*, only the above–mentioned parameters influence the qualitative aspects of the growth of the product phase.

For \( \delta T \) just below the first–order transition temperature \( T_1 \), the profile in Fig. 6 develops. This type of dynamical evolution has been called a “two–kink” growth front — also see Fig. 1 of Ref. [4]. Here we utilize the evolution shown in Fig. 6a to develop an approximation
for the growth interface found in this temperature regime. This approximation provides us with an excellent model from which an accurate theory of the instability of this interface can be fully developed.

Consider the representation of the displacement field shown in Fig. 7. The similarity to the growth interface of Fig. 6a for \( x > 20 \) is clear. For simplicity, we have shifted the “back end” of the interface to be at \( x = 0 \), as well as reflecting the displacement field to be positive in the region of interest. We do not possess an analytical expression for this interface profile, and thus it is necessary to approximate its functional form. This is accomplished by ignoring the “smoothing” imposed by the strain gradients; this leads to the following piecewise continuous function for \( u(x, t) \) [19]:

\[
u(x, t) = \begin{cases} 
0 & , x = 0 \\
e_m x & , 0 \leq x \leq vt \\
(e_m + e_2)v t - e_2 x & , vt \leq x \leq v_s t \\
0 & , x \geq v_s t 
\end{cases}
\]

In this expression, \( e_m \) is the martensitic strain, \( e_2 \) is the strain of the interface, and the speeds \( v \) and \( v_s \) will be described and related below.

The physical constraint that the interface be coherent at \( x = v_s t \) results in the following important relation between the speed \( v \) and the speed of sound \( v_s \) (see below), viz.,

\[
v = \frac{e_2}{(e_m + e_2)v_s}
\]

This one relationship, plus the analytical evaluation of \( e_m \) (already available in Eq. (16)), \( v \) and \( v_s \), will allow for all of the following analysis.

An illustrative limiting case of Eq. (32) occurs when one considers \( \Lambda \to 0 \). This implies that the speed of sound \( v_s \) becomes infinite, and thus Eq. (32) requires that \( e_2 = 0 \). This situation can be understood as the overdamped TDGLT limit of the two–kink solution [4]. It corresponds to a kink–type propagating solitary wave of amplitude \( \pm e_m \) moving to the right/left at a speed \( v \). This corresponding analytical solution has already been found by Gordon [21] and has the following form:
\[ e(x, t) = \frac{\pm e_m}{(1 + \exp[(x - vt)/\ell])^{1/2}} \] (33)

where the speed \( v \) and \( \ell \) are uniquely determined by the undercooling \( \delta T \).

Unfortunately, this solution is entirely unphysical. (This is an important point since discussions in the literature have used such a state as a model of martensitic domain wall propagation under the name of the Eshelby model.) The finite propagation time of the elastic field for the physically relevant scenario of \( \Lambda \neq 0 \) immediately suggests that such motion must have an unbounded kinetic energy \([4]\). For example, if one calculates the kinetic energy \( K \) of Eq. (33) using Eq. (4) for a system of length \( L \) one finds that \( K \propto L \), a result that simply reflects the fact that for this propagating interface the entire system is moving! Clearly, this high energy state is never going to be selected as the path through which the system approaches its steady state. Thus, the unphysical result contained in Eq. (33) serves to emphasize the importance of including the inertia of the displacement field in any accounting of the interfacial dynamics of martensitic growth fronts \([4]\). With this in mind, we return to the physically relevant \( \Lambda \neq 0 \) problem.

We wish to describe the interface displayed in Fig. 6a, and to this end we note that the complete analytical characterization of this propagating interface requires the evaluation of the speed of sound \( v_s \), possibly nonlinear, and the forward kink amplitude \( e_2 \). Note that in the moving interface portion of Fig. 7, \( v_s \) characterized the motion in the small strain \( (e_2) \) region, and for this reason we evaluate \( v_s \) by determining the nonlinear speed of sound. In a linear theory, the elastic field propagates at a characteristic velocity determined by the undercooling \( \delta T \) and mass density \( \Lambda \), \textit{viz.},

\[ v_s^2 = \frac{\delta T}{\Lambda} \] (34)

We require an expression for the nonlinear speed of sound, and to this end we consider the “nonlinear corrections” to Eq. (34), \textit{viz.},

\[ v_s^2 = \frac{\delta T + ae^2 + be^4 + \cdots}{\Lambda} \] (35)
where $a, b, \ldots$, are temperature independent constants and, by symmetry, we have only included the even powers of the strain $e$. Then, we turn to the local, nondispersive equation of motion for the strain field which can be written as

$$\partial_t^2 e = \frac{1}{\Lambda} \partial_x^2 [ (\delta T - e^2 + e^4)e] .$$  \hspace{1cm} (36)

Locally, the term $(\delta T - e^2 + e^4)$, approximately corresponds to the nonlinear force constant in the parent phase, which we will denote as $\tilde{c}$. Comparing Eq. (35) and Eq. (36) we see that if $a = -1$ and $b = 1$,

$$v_s^2 = \frac{\tilde{c}}{\Lambda} \approx \frac{1}{\Lambda} (\delta T - e^2 + e^4)$$  \hspace{1cm} (37)

represents the 4–th order nonlinear corrections to the speed of sound of an elastic wave of amplitude $e$. In particular, for the nonlinear speed of sound $v_s$ of the strain amplitude $e_2$ interface, we shall use

$$v_s \approx \sqrt{\frac{1}{\Lambda} (\delta T - e_2^2 + e_2^4)} .$$  \hspace{1cm} (38)

The last quantity that we need to determine is the amplitude $e_2$ of the forward kink. A physically motivated method for obtaining this quantity relies on energy considerations. According to the Lagrangian dynamical formalism [8], the time rate of change of the energy $E$ of the system is related to the dissipation function $R$ by

$$\partial_t E = -2R .$$  \hspace{1cm} (39)

Thus, in order for us to derive an expression for $e_2$ we need construct the total energy $E$ of the system and the dissipation function $R$.

The energy of the system is readily calculated by using our approximation for the displacement field $u(x, t)$, viz., Eq. (31), and the following expression for the total energy density $\mathcal{E}$:

$$\mathcal{E} = \frac{1}{2} \Lambda (\partial_t u)^2 + \left( \frac{1}{2} \delta T e^2 - \frac{1}{4} e^4 + \frac{1}{6} e^6 \right) .$$  \hspace{1cm} (40)
The total energy is then simply the piecewise spatial integration of the above equation over the regions $I_1 = [0, vt]$, and $I_2 = [vt, v_s t]$. The result of such a calculation yields an expression for $E$, viz.,

$$
E = \frac{e_m e_2 v_s}{(e_m + e_2)} \left[ \delta T e_2 - \frac{3}{4} e_2^3 + \frac{2}{3} e_2^5 + \frac{1}{2} \delta T e_m - \frac{1}{4} e_m^3 + \frac{1}{6} e_m^5 \right] t ,
$$

and $\partial_t E$ is given by a single time derivative of the above equation.

Using the same procedure as in [4], we approximately solve for the dissipation function through the use of the analytical expression for the overdamped kink, viz., Eq. (33). At long times, the dissipation function can be written as [4],

$$
R \approx \frac{e_m^2}{16 \ell v^2}
$$

where $v$ is the growth speed and $\ell$ is a measure of the interfacial width ($\ell \sim 1$ domain wall width). The energy balance condition, Eq. (39), can now be restated in terms of the only, a priori, unknown quantity, namely $e_2$, viz.,

$$
\frac{e_m e_2 v_s}{(e_m + e_2)} \left[ \delta T e_2 - \frac{3}{4} e_2^3 + \frac{2}{3} e_2^5 + \frac{1}{2} \delta T e_m - \frac{1}{4} e_m^3 + \frac{1}{6} e_m^5 \right] - \frac{e_m^2}{8 \ell v^2} = 0 ,
$$

where it should be recalled that $v_s$ and $v$ can both be expressed in terms of $e_2$. We have tested this calculation by numerically solving for $e_2$ in Eq. (43) and then using this in Eq. (32) to obtain a value for $v$. We have found that for the parameters $E_W/E_B = 1$, $\Lambda = 1$, $\ell = \sqrt{3}/(2 e_m^2)$, $v = 0.035$, which compares superbly with the value found from the numerical integration of the full dynamical equations, viz., $v_{num} = 0.033$. Similar favourable comparisons are found for other choices of $\delta T$ and $\Lambda$ [20]. This excellent agreement between the analytical and numerical values for the growth speed $v$ clearly justifies the approximation that we have used for $u(x, t)$ in Eq. (31).

One may relate this speed to that in the proper, 1st–order, ferroelastic transition undergone by Lanthanum. One predicts that the two–kink interfacial speed would be of the order of 10% (or less) of the smallest speed of sound, namely about 80 m/s.

We have found that this interfacial motion does not persist — instead, as the temperature of the system is lowered a second type of propagating growth front develops. Figure 8
illustrates a typical solution for both the displacement and strain fields. The strain figure makes clear the fascinating physics that Bales and one of us [4] observed. This growth front has been called “dynamical twin formation” [4] because the moving interface separating product from parent phase leaves behind an alternating structure consisting of both doubly degenerate low-temperature variants — these are so-called martensitic twins, and in Fig. 8c we display the steady-state profile of a short twinned crystal that results from the dynamics shown in Figs. 8a/b.

Below we shall describe the origin of this interfacial motion. However, here we make one straightforward observation contrasting this type of interfacial motion with that of Fig. 8. Figure 8 shows a snapshot of the kinetic energy density, $\tilde{K}(x, t)$, for the dynamical twinning solution at time $t = 360$ scaled time units, and illustrates the dramatic localization of the kinetic energy density around the interface ($x \approx 75$) of the transformation front. This is clearly different from the entirely delocalized kinetic energy density found throughout the $e_2$ interface shown in Fig. 10 (also $t = 360$ scaled time units) — note the very different scales of these two figures.

Both growth profiles can be understood as arising from the finite propagation time of the elastic field found for $\Lambda \neq 0$. Recall that in our approach sound waves always propagate at sufficiently long wavelengths. It then follows that the displacement field far from the interface must remain fixed, and thus there is an induced stress in the immediate vicinity of the growth front; that is, the parent phase is bent locally at the interface. The magnitude of the stress induced in the parent phase depends strongly on the material parameters, $\Lambda$ and $\delta T$, through Eq. (32). So, as the growth speed approaches the speed of sound, the $e_2$ strain increases and will eventually exceed the spinodal strain [23] determined by $\partial^2 f_L(e)/\partial e^2 = 0$, viz. ,

$$e_{ss} = \sqrt{0.1(3 - \sqrt{9 - 20\delta T})}.$$ (44)

When this occurs the (local) interface becomes unstable and a dynamical phase transition arises producing a new type of interfacial motion, viz. that shown in Fig. 8a/b. Summariz-
ing, we see that the dynamical twinning shown in Fig. 8a/b is a consequence of the local instability of the $e_2$–strain interface of Fig. 6 a/b separating product from parent phase. It is worthwhile to re–emphasize that although the $t = 0$ initial states discussed in this paper were twinned nuclei, the dynamical evolutions illustrated in Fig. 6 and Fig. 8 are independent of the initial displacement field (e.g., see also Fig. 1 and 2 of [4] where different initial conditions were used).

Based on the above, one can expect that in $(\Lambda, \delta T)$ phase space, a twinning/no–twinning phase diagram may be constructed. By setting $e_2 = e_{ss}$ in Eq. (13) and substituting Eq. (32) in for $v$, we can solve for the critical value $\Lambda_c(\delta T)$ [24], viz.,

$$
\Lambda_c^{1/2} = \frac{-e_m^3 e_{ss}(\delta T - e_{ss}^2 + e_{ss}^4)^{1/2}}{4\sqrt{3}(e_m + e_{ss})(\delta T e_{ss} - \frac{3}{2} e_{ss}^3 + \frac{2}{3} e_{ss}^5 + \frac{1}{2} \delta T e_m - \frac{1}{4} e_m^3 + \frac{1}{6} e_m^5)},
$$

(45)

where it is to be recalled that both $e_m$ and $e_{ss}$ are explicit functions of $\delta T$ through Eqs. (16,44); viewed in $(\Lambda, \delta T)$ phase space, this trajectory defines the critical value of $\Lambda$ at which twinning occurs. This curve is plotted in Fig. 11 along with the results from the numerics. The divergence of Eq. (45) when $\delta T \sim 0.136$ defines the range of undercoolings for which twinning will not occur for any value of $\Lambda$. The superb agreement of Eq. (45) with that of our numerics clearly justifies our theory of the instability of the growth interface.

5. SUMMARY AND DISCUSSION:

We have presented an exhaustive study of the dynamical nucleation and growth in a one–dimensional version of a first–order, shear elastic martensitic phase transformation. Our approach involves treating nonlinear elastic models of these transitions as nonconvective, hydrodynamic systems. We have been able to determine for the first time that the bulk critical nuclei of the system are twinned structures. We have obtained approximate analytical expressions for these structures, and a comparison of Fig. 3b and Fig. 5 shows that our results are in superb agreement with the exact numerical solutions. In addition, we have exactly solved for the critical nucleus of a finite, but large system with open boundary
conditions, viz., Eqs. (17,18,19). We have shown that, for this case, the critical nucleus is a localized surface state with (almost) exactly $1/4$ the energy of the bulk critical nucleus. We conclude that surface nucleation is the dominant route for the formation of martensite, at least in the absence of impurities.

A full treatment of the martensitic growth dynamics associated with supercritical nuclei has also been presented. A phase diagram connecting the rescaled mass coefficient $\Lambda$ and the undercooling $\delta T$ has been derived. We have shown that the transformation fronts propagate through the system with a speed given by Eq. (32).

The extension of our work to higher dimensions is in principle relatively straightforward. In fact, a large amount of numerical work examining a triangular–to–oblique transition has already been completed. The formal ingredients are the same as the one–dimensional model, except that the numerical analysis becomes much more difficult — the restrictions to higher dimensional systems are essentially technical ones. New integration software will be needed in order to fully investigate the dynamical evolution of such systems. Analytical work will be, obviously, greatly complicated.

Although extending our one–dimensional phenomenology to completely general 2D and 3D systems can pose substantial technical problems, we have had much success in looking at higher dimensional models with special symmetries. In particular, we have been able to use the same methodology as in our 1D studies to investigate change of volume first–order transitions in a $d$–dimensional, nonlinear, nonlocal elastic system ($d = 1, 2, \ldots, \infty$). In these models, the system is reduced down to $1+1$ dimensions for which the variant method of lines and Lagrangian formalism presented in this paper are directly applicable in all $d$–dimensions. For these systems we find that only surface nuclei exist, and that all dynamical evolutions of the system to steady state pass through such nuclei — these results will be presented elsewhere.
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Following the notation of Ref. [10], let \( u \) be the displacement at any position in space, and assume that

\[
u = f(W_1, W_2, ..., W_{10}) \tag{A1}\]

where

\[W_1 = A, \text{ some positive constant of dimension } [A] = \frac{m \ell}{\theta \tau^2},\]

\[W_2 = B, \text{ some positive constant of dimension } [B] = \frac{m \ell}{\tau},\]

\[W_3 = C, \text{ some positive constant of dimension } [C] = [B],\]

\[W_4 = D, \text{ some positive constant of dimension } [D] = \frac{m \ell^3}{\tau^2},\]

\[W_5 = \gamma, \text{ the sound wave viscosity of dimension } [\gamma] = \frac{m \ell}{\tau},\]

\[W_6 = \rho, \text{ the linear mass density of dimension } [\rho] = \frac{m}{\ell},\]

\[W_7 = \delta T, \text{ the undercooling of dimension } [\delta T] = \theta,\]

\[W_8 = L, \text{ the system size of dimension } [L] = \ell\]

\[W_9 = x, \text{ the distance along the bar of dimension } [x] = \ell,\]

\[W_{10} = t, \text{ the elapsed time after an initial strain is applied of dimension } [t] = \tau.\]

For this analysis, we have used dynamical units as our fundamental basis, viz.,

\[L_1 = \ell \text{ (length)}\]

\[L_2 = m \text{ (mass)}\]

\[L_3 = \tau \text{ (time)}\]

\[L_4 = \theta \text{ (temperature)}\]

The corresponding dimension matrix is then simply:

\[
\mathbf{B} = \begin{bmatrix}
1 & 1 & 1 & 3 & 1 & -1 & 0 & 1 & 1 & 0 \\
1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\
-2 & -2 & -2 & -2 & -1 & 0 & 0 & 0 & 1 \\
-1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0
\end{bmatrix} \tag{A2}
\]

This matrix has a rank \( r(\mathbf{B}) = 4 \), whence by the Buckingham Pi–Theorem [10], the number of measurable dimensionless quantities, under our choice of fundamental units, is
\[ k = n - r(B) = 10 - 4 = 6 \], where \( n \) is the total number of independent variables and constants appearing in the system. It also follows from the Buckingham Pi–Theorem that our system can be re–expressed in dimensionless form where \( \pi = \tilde{u}(\Omega) \) is a dimensionless dependent variable and \( \Omega = \{\pi_1, \pi_2, \ldots, \pi_k\} \) are dimensionless independent variables and dimensionless constants. The exact form of these \( k \) dimensionless quantities can be found by solving for the null space of the dimension matrix \( B \). The dimensionless displacement field \( \tilde{u}(\Omega) \) is found by solving the linear system \( By = -a \), where \( a \) is the dimension vector of \( u \). Tedious algebra reveals that \( \Omega \) and \( \pi \) can be written as

\[
\begin{align*}
\pi_1 &= \frac{B}{\gamma} t, \\
\pi_2 &= \left[ \frac{B}{D} \right]^{1/2} x, \\
\pi_3 &= \left[ \frac{B}{D} \right]^{1/2} L, \\
\pi_4 &= \frac{A}{B} \delta T, \\
\pi_5 &= \frac{\rho D}{\gamma^2}, \\
\pi_6 &= \left[ \frac{C}{B} \right]^{1/2},
\end{align*}
\]

(A3)

and

\[
\pi = \left[ \frac{B}{D} \right]^{1/2} u .
\]

(A4)

If we identify \( \pi_5 = \Lambda \), a rescaled mass coefficient, and rescale \( \pi_1, \ldots, \pi_4 \) using \( \pi_6 \), we arrive at the following dimensionless, rescaled independent variables and constants,

\[
\begin{align*}
\tilde{t} &= \frac{\pi_1}{\pi_2^2} = \frac{B^2}{\gamma C} t, \\
\tilde{x} &= \frac{\pi_2}{\pi_6} = \frac{B}{\sqrt{CD}} x, \\
\tilde{L} &= \frac{\pi_3}{\pi_6} = \frac{B}{\sqrt{CD}} L, \\
\delta \tilde{T} &= \pi_6^2 \pi_4 = \frac{AC}{B^2} \delta T, \\
\frac{\rho D}{\gamma^2} &= \Lambda .
\end{align*}
\]

(A5)

These scaled quantities, along with Eq. \( \text{(A4)} \), can now be used in Eqs. \( \text{(6)}, \text{(7)} \) and \( \text{(8)} \), to obtain a complete two–parameter model which depends only on a rescaled undercooling \( (\delta \tilde{T}) \) and a rescaled mass coefficient \( (\Lambda) \), \textit{viz},

\[
\Lambda (\partial_x^2 \tilde{u}) = (\partial_x^2 \tilde{u}) \left[ \delta \tilde{T} - 3(\partial_x \tilde{u})^2 + 5(\partial_x \tilde{u})^4 \right] - (\partial_x^4 \tilde{u}) + (\partial_t \partial_x^2 \tilde{u}) ,
\]

(A7)

with boundary conditions at \( \tilde{x} = \pm \frac{\tilde{L}}{2} \),

\[
\delta \tilde{T}(\partial_x \tilde{u}) - (\partial_x \tilde{u})^3 + (\partial_x \tilde{u})^5 + (\partial_x \partial_t \tilde{u}) - (\partial_x^3 \tilde{u}) = 0,
\]

(A8)

\[
(\partial_x^2 \tilde{u}) = 0 .
\]

(A9)
APPENDIX B: EXACT SOLUTIONS FOR AN INFINITE DOMAIN:

In terms of the shear strain, the bulk, zero–force equation that we wish to solve for is given by

\[ \partial_x^2 e - (\delta T e - e^3 + e^5) = 0 \] (B1)

where the boundary conditions are \( \partial_j e(x) = 0 \) at \( x = \pm \infty \) and \( j = 0, 1, ..., 4 \).

If we multiply Eq. (B1) by \( \partial_x e \) and integrate, we obtain

\[ (\partial_x e)^2 - (\delta T e^2 - \frac{1}{2}e^4 + \frac{1}{3}e^6) = c \] (B2)

where \( c \) is an integration constant. From the constraint that all derivatives of the strain must vanish at \( \pm \infty \), it follows that \( c = 0 \).

Let \( e = \pm 1/\sqrt{w} \), so that we are now looking for singular solutions of \( w \). Note that this transformation is well defined because \( e(x) \) is bounded for all \( x \in (-\infty, \infty) \). Equation (B2), with \( c = 0 \), then becomes:

\[ (\partial_x w)^2 - (4\delta T w^2 - 2w + \frac{4}{3}) = 0 \] (B3)

Re–writing this as an integral over \( w \) and \( x \), we have,

\[ \int \frac{dw}{\sqrt{4\delta T w^2 - 2w + \frac{4}{3}}} = \int dx \] (B4)

Both the left and right hand sides of Eq. (B4) can be evaluated exactly to give the following expression for \( w \) and \( x \)

\[ \ln(-1 + 4\delta T w + \sqrt{\frac{8\delta T}{3} \sqrt{2 - 3w + 6\delta T w^2}}) = x - x_0 \] (B5)

where \( x_0 \) is an integration constant. The inversion of this equation will yield \( w \) as a function of \( x \), viz,

\[ w(x) = \frac{3 - 16\delta T + 6 \exp[2\sqrt{\delta T}(x - x_0)] + 3 \exp[4\sqrt{\delta T}(x - x_0)]}{24\delta T \exp[2\sqrt{\delta T}(x - x_0)]} \] (B6)
Solutions to Eq. (B1) are finally obtained by recalling that $e = \pm 1/\sqrt{w}$, whence,

$$e_0(x - x_0) = \pm 2\sqrt{6\delta T} \frac{\exp[2\sqrt{\delta T}(x - x_0)]}{\sqrt{3 - 16\delta T + 6 \exp[2\sqrt{\delta T}(x - x_0)] + 3 \exp[4\sqrt{\delta T}(x - x_0)]}} \quad (B7)$$

A direct substitution of Eq. (B7) into Eq. (17) confirms that they are indeed zero–force solutions.
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[24] This equation corrects some typographical errors in the analogous equation in Ref. [4].
FIGURES

FIG. 1. A plot of the local elastic free–energy density, $f_L(e)$, of Eq. (1) for $A = B = C = 1$ (corresponding to the scaled units used in our nucleation and growth studies) and $\delta T = 1/6$. The barrier height is denoted by $E_B$ and the well depth by $E_W$.

FIG. 2. The classical nucleus (long–dash line), corresponding to $n \to \infty$ in Eq. (21), and a Gaussian fluctuation (dot–dashed line) corresponding to $n = 1$. Again referring to Eq. (21), for these figures $d = 10$ and $u_0 = 1$.

FIG. 3. (a) The bulk critical nucleus found from solutions to Eqs. (17,18,19) for $E_W/E_B = 0.2, 1/6$, and 5 — the tallest curve corresponds to the smallest ratio of $E_W/E_B$. (b) The bulk critical nucleus in strain space for the ratio $E_W/E_B = 1.0$.

FIG. 4. A plot of Eq. (25) for $E_W/E_B = 1.0$. This curve has been shifted so that $x = 0$ corresponds to the $x_{max}$ given in Eq. (26).

FIG. 5. A plot of the analytical approximation to the critical nucleus for $E_W/E_B = 1.0$ based on Eq. (27) using the procedure described in the text for evaluating $x_0$. This strain profile should be compared with that shown in Fig. 3b, the (numerically determined) exact critical nucleus for this temperature.

FIG. 6. (a) Evolution of the displacement field for a supercritical nucleus ($\epsilon = +0.01$ in Eq. (23)) for $E_W/E_B = 1.0$. The dashed line is the (static) initial displacement field, and the solid lines show how the system progresses at the times $t = 0$, 180, 220, 260 and 300. (b) Evolution of the strain field for the supercritical nucleus studied in (a); $e_m$ is the martensite strain given by Eq. (16). The dashed line is the (static) initial strain field, and the solid lines show how the system progresses at the times $t = 0$, 400, 500 and 600. (c) The steady–state $t \to \infty$ profiles of the displacement field (solid line) and the strain field (dashed line). In the context of our model, this steady state corresponds to a single twin or “bicrystal”.

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FIG. 7. An idealized representation of the two–kink growth interface. For the $t = 0$ state being the dashed line, the solid line shows the interface at some later time $t$. $v$ is the interfacial growth speed and $v_s$ is the nonlinear speed of sound, a quantity that we have attempted to evaluate in Eq. (38). The exclusion of the nonlocal term, viz., $\partial^4_x u$, simplifies the problem to finding only a $C^1$ function for $u(x,t)$.

FIG. 8. (a) Evolution of the displacement field for a supercritical nucleus ($\epsilon = +0.01$ in Eq. (23)) for $E_W/E_B = 6.5$. The dot–dashed line is the (static) initial displacement field, and the long–dashed line corresponds to a time of $t = 360$, and the solid line represents a time of $t = 720$. (b) Evolution of the strain field for the supercritical nucleus studied in (a); $e_m$ is the martensite strain given by Eq. (16). (c) The steady–state $t \to \infty$ profiles of the displacement field (solid line) and the strain field (dashed line). In the context of our model, this steady state corresponds to a polytwinned crystal.

FIG. 9. The kinetic energy density for the dynamical twinning growth front at $t = 360$ for $E_W/E_B = 6.5$. For $x \gtrsim 75$, the kinetic energy density is almost completely localized (see text).

FIG. 10. The kinetic energy density for the two–kink growth front at $t = 360$ for $E_W/E_B = 1.0$. For $x \gtrsim 75$, the kinetic energy density is spread out over the $e_2$ growth interface.

FIG. 11. The renormalized mass density, $\Lambda$, as a function of the undercooling $\delta T$. The region labeled $(I)$ corresponds to those values of $(\Lambda, \delta T)$ for which twinning will occur. Region $(II)$ will only result in the two–kink profile shown in Fig. 6a/b. $\delta T_1 = 0.1875$ is the transition temperature in scaled units. The solid circles are the numerical data of Ref. [4].
