Field Dislocation Mechanics and Phase Field Crystal models

Amit Acharya

Department of Civil and Environmental Engineering,

and Center for Nonlinear Analysis, Carnegie Mellon University,

Pittsburgh, Pennsylvania 15213, USA

Jorge Viñals

School of Physics and Astronomy, University of Minnesota,

Minneapolis, Minnesota 55455, USA

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Abstract

A formulation of the Phase Field Crystal model is presented that is consistent with the necessary microscopic independence between the phase field, reflecting the broken symmetry of the phase, and both mass density and elastic distortion. Although these quantities are related in equilibrium through a macroscopic equation of state, they are independent variables in the free energy, and can be independently varied in evaluating the dissipation functional that leads to some of the model governing equations. The equations obtained describe dislocation motion in an elastically stressed solid, and serve as an extension of the equations of dislocation mechanics to the Phase Field Crystal setting. Both finite and small deformation theories are considered, and the corresponding kinetic equations for the fields derived.

I. INTRODUCTION

The Phase Field Crystal (PFC) model has been introduced as a mesoscale description of a nonequilibrium crystalline phase, valid at the molecular length scale, but only over long, diffusive time scales [1]. By eliminating the need to resolve the time scale associated with lattice vibration, the Phase Field Crystal model has become a widely used computational tool capable of describing a wide variety of phenomena in materials science [2]. One of the strengths of the formulation is the ease in the description of defected solids, including, for example, dislocation dissociation, stacking fault formation, grain boundary motion, and coarsening of polycrystalline configurations. Further spatial coarse graining has also been undertaken, leading to models in which the characteristic spatial variation is also slow compared with the molecular length scale [3–6].

The Phase Field Crystal model begins with the introduction of a phenomenological, non convex free energy functional, $\Phi_{sh}[\psi]$, of a phase field $\psi(\mathbf{x}, t)$ and of its gradients. The choice of nonlinearity in Φ_{sh} determines the symmetry of the resulting ground state lattice. While the bulk of the early work focused on two dimensional hexagonal lattices, research has also considered three dimensional systems, including fcc and bcc lattices [4], and specific materials such as, for example, Fe [7] or graphene [8]. We assume here that $\Phi_{sh}[\psi]$ is given for a specific three dimensional system, except in Sec. III A in which we discuss the application of our analysis to a two dimensional hexagonal lattice.

Phase Field Crystal model free energies have been derived by using Density Functional

Theory methods, with the expectation of obtaining functionals that capture the long time diffusive evolution of the mass density as the relevant order parameter [9, 10]. The free energies obtained provide a reasonable description of the freezing phase transition [11]. However, extensions to include the momentum density in the set of slow or hydrodynamic variables have not been considered to the same extent, except for colloidal systems [12], and, more recently, in the so called hydrodynamic formulation of the Phase Field Crystal [13]. In this latter analysis, both mass and momentum conservation are considered at the mesoscale. For weak lattice distortions around the ground state a smooth displacement field can be introduced, related to the phase of ψ. A dynamical dispersion relation can be derived that includes both phonon propagation and damping, in agreement with standard theory. Notably, the dispersion at large wavenumbers becomes entirely diffusive as diffusion of the phase field controls the local relaxation of the weakly distorted configuration. Although this study does not address how to explicitly incorporate topological constraints necessary to describe a defected lattice, results are given for grain rotation and shrinkage in a two dimensional, hexagonal phase. Grain radius is seen to decay with time as $t^{-1/2}$, as expected. The amplitude of the decay rate increases with increasing Newtonian viscosity in the momentum equation. In the limit of large viscosity, the results of the overdamped model of Ref. [14] for the grain size as a function of time are recovered. Since the boundary of the grain comprises a periodic array of dislocations, this example indicates that the theory is capable of describing the evolution of an initially defected configuration.

However, the Phase Field Crystal model has some important shortcomings that point to its incompleteness. In most research to date, the mass density and lattice distortion of the crystalline phase are generally described by the same scalar field ψ. In this case, their variations are not independent. Consider, for example, that ψ is a conserved mass density. Then, its local variation through distortion is $\delta\psi = -\partial_k(\psi\delta u_k)$, where u_k is the k-th component of the displacement vector, the phase of ψ. From this relation, the variation $\delta\Phi_{sh}/\delta u_k = \psi\partial_k(\delta\Phi_{sh}/\delta\psi)$ follows. Since the stress is defined through $\partial_j T_{ij} = -\delta\Phi_{sh}/\delta u_i$, then $\partial_j T_{ij} = -\psi\partial_i(\delta\Phi_{sh}/\delta\psi)$. This relation is correct in equilibrium where both sides of the equation vanish, but not in general outside of equilibrium. Furthermore, if both variations are not considered to be independent, then lattice distortions can only relax diffusively, which is unphysical. This difficulty has been recognized for a long time, and a number of modified models have been introduced to allow for relaxation of the phase field in a time

scale faster than diffusion [14–17], including the hydrodynamic formulation alluded to above [13].

Despite these modifications to the Phase Field Crystal model in order to accelerate the relaxation of elastic distortions, restricting the model to a single field ψ still leads to difficulties or inconsistencies. One such difficulty involves the definition of physical system boundaries, and the imposition of boundary conditions involving changes in domain shape or traction. The specification of boundary traction, for example, needs to be done indirectly through manipulation of the phase field. In their study of the motion of a single dislocation under an imposed strain, Berry et al. [18] rigidly displaced a small layer of sites at the boundary. The resulting distortion propagated into the bulk system slowly (diffusively), thus preventing direct control of the stress field in the defect region other than readjusting the displacement of the boundary layer, and waiting for a long time until the bulk stress would readjust. The ensuing motion of the dislocation is quite different from would be expected from classical elasticity and the Peach-Köhler force [19, 20]. A second and related issue is that in processes involving time evolution with exchange of mechanical power through the boundary of a body, purely elastic processes are possible that involve no dissipation of energy. However, the classical phase field evolution necessarily involves dissipation of energy and therefore cannot be correct for the modeling of elasticity (both in the presence or absence of defects) if the modeling of elasticity is tied directly to the evolution of the phase field. A third issue concerns the recent result that the ground state of the Phase Field Crystal appears to be, in fact, under a large pressure. For example, for the model parameters that are employed to describe bcc Fe, the ground state pressure is as large as 1.8×10^6 atm at melting [7]. Whether this state of pressure is or is not taken into account in the determination of the linear elastic constants from the phase field free energy, it is possible to predict both a decrease or an increase in their values as a function of the spatial average of ψ, $\overline{\psi}$ (related to average density or pressure) [21]. The proper definition of strain from the phase field has been further discussed in Ref. [8] which suggests holding the value of $\overline{\psi}$ constant under volume change, which implies that it is not related to the mass density. Finally, modeling plastic motion of defects within the Phase Field Crystal leads to another class of difficulties. Elastic and plastic distortions are independent, and ordinarily relax over widely different time scales. While it is well understood that mass and lattice defect velocities are independent quantities [22], they are simultaneously described

by a single scalar quantity ψ in the Phase Field Crystal model.

We also mention related work on Phase Field models of dislocation motion [23–30] that have been quite successful in solving a variety of problems related to dislocation mechanics close to equilibrium. In this class of models, the phase field does not represent a mass density but rather accounts directly for defect slip. The models are mostly restricted to small deformation kinematics, and are based on the classical notion of plastic strain from a fixed reference configuration (that is, strain not physically determinable from an internally stressed defected initial state). More importantly, Phase Field models require the definition of the so-called 'crystalline energy' or the 'Generalized Stacking Fault energy' that has to be defined from some a-priori knowledge of the slip-systems of a material, and involve an atomistic γ-surface procedure (first introduced by Vitek in [31]). As a consequence, the number of independent phase fields included in the model is related to the number of slip systems identified and considered [26, 28], and dislocation combination rules need to be adapted accordingly [25]. This is different from the PFC which *predicts* both material symmetry and defect motion on preferred planes and directions that are dictated by that symmetry [32]. Furthermore, the dynamics of Phase Field models rely on an Allen-Cahn type gradient flow for a set of non conserved phase fields. This is a non-convex incremental energy minimization with highly non-unique (even locally in time) solutions as shown in [24]. One consequence of a gradient flow kinetics is that the phase field can evolve in a local region where it is spatially homogeneous, purely based on the levels of stress and energy density fields. This is in contrast, for example, to Field Dislocation Mechanics (FDM, described below) in which evolution of the elastic distortion (beyond 'convection') can only occur at a field point where a dislocation exists (i.e., the curl of the distortion does not vanish), regardless of the level of stress or energy density at that point. This 'thermodynamic driving force' property follows from the second law of thermodynamics constrained by an explicit condition of conservation of Burgers vector (topological charge) during the evolution of elastic distortion - and is a feature that is consistent with the form of the Peach-Köhler force of classical dislocation theory.

The approach that we propose here is based on the realization that a PFC (or Brazovskii/Swift-Hohenberg) functional does not posses intrinsic elasticity. The Brazovskii functional, originally derived to describe the phase transition to a generic modulated phase, has been widely used in many disparate fields in which a modulated structure spontaneously forms.

However, despite its elegance and generality, it contains no information on the microscopic forces that hold matter together, and hence on macroscopic elastic response. This observation is borne out by the fitting it requires in practice, see, e.g., [8, Eqn. (65)]. Therefore, in the present context we consider the phase field to be a mathematical device or indicator function that (i) describes the symmetry of a crystalline lattice even when locally deformed, (ii) serves to locate topological defects and provides for their topological index, and, (iii) allows to conserve topological charge in processes involving defect motion close to equilibrium through its 'phase' being constrained to equal a field (described below) with mechanics that explicitly satisfies a conservation law for (signed) topological charge, while also allowing defect nucleation and annihilation. Our model is based on the introduction of a configurational distortion tensor $\boldsymbol{P}$, a pointwise functional of the phase field ψ, which coincides with the inverse elastic distortion tensor of the medium $\boldsymbol{W}$ only in equilibrium. Away from equilibrium, we allow relative fluctuations between both such that the elastic response is captured by $\boldsymbol{W}$, and the diffusive relaxation by $\boldsymbol{P}$.

The fully nonlinear (geometric and material) dynamics of the independent inverse elastic distortion field $\boldsymbol{W}$ is governed by Field Dislocation Mechanics (FDM) [33–39]. FDM completes the program of the theory of continuously distributed dislocations [40, and earlier references therein], [22, 41–46] extended from its origins in linear elasticity, and in links between differential geometry and defect kinematics, to a full-fledged nonlinear theory of continuum mechanics. FDM includes equations of balance and defect kinematics, and allows large irreversible material deformations (plasticity) with both inertia and dissipation. It can treat geometric and material nonlinearity in finite bodies of arbitrary elastic anisotropy, subjected to general boundary and initial conditions. The level of description is also suitable for computer implementation to obtain approximate solutions [38, 47], [48, and following works for the geometrically linear model]. FDM is 'fluid-like' (or Eulerian) in its description of the behavior of solids with defects as it does not rely on the existence of a reference configuration of the body, or a plastic distortion tensor (consistent with the behavior of an atomistic assembly). Yet it can predict physically observed large, irreversible plastic deformation of the body due to the motion of dislocations, as well as recoverable elastic deformation and residual stress. The coupled FDM-PFC model that we introduce shares all of these important properties.

II. FINITE DEFORMATION PHASE FIELD CRYSTAL THEORY OF DISLOCATION MOTION

A. Choice of fields

We focus on an isothermal system and consider a simply-connected body (even in the presence of line defects) at all times. The following set of independent variables is introduced: ρ, the continuum mass density, the material velocity $\boldsymbol{v}$, $\boldsymbol{W}$, the inverse elastic distortion, and ψ the phase field. The tensor field $\boldsymbol{W}$ maps the (linear approximation to the) deformed elastic lattice pointwise to the undeformed lattice (the latter assumed known). In the absence of line defects, $\operatorname{curl} \boldsymbol{W} = \boldsymbol{0}$ (compatible elasticity), and a potential field $\boldsymbol{X}$ exists defining a reference configuration in which the undeformed lattice can be embedded: $dX_i = \frac{\partial X_i}{\partial x_j} dx_j = F^{-1}_{ij} dx_j$, with $\boldsymbol{F}^{-1} = \boldsymbol{W}$. In terms of a displacement field $\boldsymbol{u}$ of the reference (which exists in the compatible case), the tensor $U_{ij} = \partial_j u_i = \partial_j (x_i - X_i) = \delta_{ij} - F^{-1}_{ij}$, so that $\boldsymbol{W} = \boldsymbol{F}^{-1} = \boldsymbol{I} - \boldsymbol{U}$. Even in the incompatible case, defining $\boldsymbol{W}^{-1} - \boldsymbol{I} = \boldsymbol{U}$ and assuming $|\boldsymbol{U}| \ll 1$, $\boldsymbol{W} \approx \boldsymbol{I} - \boldsymbol{U}$.

The key ingredient of our model is a (two-point) second rank tensor $\boldsymbol{P}$ (standing for *phase*) with the same symmetry properties under rotation as $\boldsymbol{W}$. Its value at each point in the material is a functional of the phase field ψ, and is defined so as to describe the distortion of the surfaces of constant ψ. After averaging the phase field over a scale on the order of its characteristic lattice spacing, q_0^{-1} [49], one can define a triad of local wavevectors $\boldsymbol{q}^n$, different than those of the ground state of $\Phi_{sh}[\psi]$, the latter denoted by $\boldsymbol{q}_0^n$. Then we define $\boldsymbol{q}_0^n = \boldsymbol{P}^{-T} \boldsymbol{q}^n$. The tensor $\boldsymbol{P}$ describes a local configurational distortion that can be associated with the field ψ, without endowing the phase field with any elastic properties. Note that the curl of the tensor field $\boldsymbol{W}$ is not zero in general, and that $\boldsymbol{P}$ will not vanish at defects in the phase field equivalent lattice.

B. Balance equations

The density ρ satisfies mass conservation

$$\dot{\rho} + \rho \operatorname{div} \boldsymbol{v} = 0 \tag{1}$$

where $\dot{(\,)}$ represents a material time derivative, and $\boldsymbol{v}$ is the material velocity (center of mass velocity of an element of volume), and all spatial differential operators at any given time are on the configuration occupied by the body at that time. Momentum conservation is written as

$$\rho\dot{\boldsymbol{v}} = \operatorname{div}\boldsymbol{T} + \rho\boldsymbol{b} \tag{2}$$

where $\boldsymbol{T}$ is the stress tensor, which in the present context is symmetric, and $\boldsymbol{b}$ is a specified body force density (per unit mass). For quasi-static motions of the body, we simply write $\operatorname{div}\boldsymbol{T} + \rho\boldsymbol{b} = \boldsymbol{0}$.

If the medium contains dislocation lines, the inverse elastic distortion is incompatible, and we write [46]

$$\operatorname{curl}\boldsymbol{W} = \operatorname{curl}\boldsymbol{P} = -\boldsymbol{\alpha}, \tag{3}$$

where $\boldsymbol{\alpha}$ is the dislocation density tensor. This condition reflects the topological constraint that the integral of this tensor over a surface equals the sum of the Burgers' vectors of the dislocation lines that thread the surface. As introduced, $\boldsymbol{P}$ is assumed to contain the entire lattice incompatibility of the configuration ψ. Motion of the dislocation lines induces a change in the distortion tensor given by [34, 36]

$$\dot{\boldsymbol{W}} + \boldsymbol{W}\boldsymbol{L} = \boldsymbol{\alpha} \times \boldsymbol{V} \tag{4}$$

where $\boldsymbol{L} = \operatorname{grad}\boldsymbol{v}$ is the (mass) velocity gradient tensor and $\boldsymbol{V}$ is the local dislocation velocity relative to the mass velocity. This equation is implied by topological charge conservation under defect motion (up to a gradient of a vector field that can be assumed to vanish for microscopic defect motions) [50] and, conversely, enforces such conservation when operative.

C. Free energy, dissipation inequality, and governing equations

We next consider the free energy density of the system φ to be a function not only of ρ, $\boldsymbol{W}$ and ψ, but also of $\boldsymbol{P}$, treated as an independent variable,

$$\int_\Omega d\boldsymbol{x}\ \rho\varphi(\rho,\boldsymbol{W},\psi,\boldsymbol{P}) = \int_\Omega d\boldsymbol{x}\ \rho\varphi_e(\rho,\boldsymbol{W},\boldsymbol{P}) + C_{sh}\Phi_{sh}[\psi] + \\ + \frac{C_w}{2}\int_\Omega d\boldsymbol{x}\ \rho|\boldsymbol{W}-\boldsymbol{P}|^2 + \frac{C_\rho}{2}\int_\Omega d\boldsymbol{x}\ \rho(\rho-\psi)^2. \tag{5}$$

The first term on the right hand side of Eq. (5) is the standard elastic energy. We allow a dependence on $\boldsymbol{P}$ only to express the fact that the actual functional form of the elastic

constant matrix will depend on the symmetry of the lattice, and potentially on the linear elastic constants that will themselves depend on that symmetry, and the local state of distortion of the phase field. For the simplest extension of linear elasticity to rotationally invariant nonlinear elasticity, for example, one would write

$$\varphi_e = \frac{1}{2\rho_0}\boldsymbol{E} : \boldsymbol{C}(\boldsymbol{P}) : \boldsymbol{E}, \tag{6}$$

where $\boldsymbol{C}$ is the tensor of elastic moduli, possibly dependent on $\boldsymbol{P}$, and $\boldsymbol{E}$ is the symmetric strain tensor $\boldsymbol{E} = \frac{1}{2}\left(\boldsymbol{F}^{eT}\boldsymbol{F}^{e} - \boldsymbol{I}\right)$. The second term on the right hand side is the standard Phase Field Crystal energy density defining the model as described in the introduction, the functional form of which depends on the symmetry of the lattice under investigation. The third and fourth terms energetically penalize the difference between representations of the (inverse) elastic distortion measures and the phase field configurational distortion, and mass density deviations, respectively. We will better motivate these two constraints after deriving the dynamical equations of the complete model, and the physical effects introduced by the constraints.

For simplicity, we introduce the notation

$$\Phi_{wp} = \int_\Omega d\boldsymbol{x}\ \rho\varphi_e(\rho, \boldsymbol{W}, \boldsymbol{P}) + \frac{C_w}{2}\int_\Omega d\boldsymbol{x}\ \rho|\boldsymbol{W} - \boldsymbol{P}|^2, \tag{7}$$

which is also, implicitly, a functional of the phase field ψ (through $\boldsymbol{P}$). The coupling constants C_{sh}, C_w and C_ρ are non negative, and we will typically focus on the case in which C_w, C_{sh} are large ($\gg |\boldsymbol{C}|$).

Motivated by Eq. (7) and the evolution of $\boldsymbol{P}$ necessary for response due to a superposed rigid motion on a given motion of a body in which ψ does not evolve, we assume that

$$\int_\Omega d\boldsymbol{x}\ \frac{\delta\Phi_{wp}}{\delta\psi}\dot{\psi} = \int_\Omega d\boldsymbol{x}\ \rho\frac{\partial}{\partial\boldsymbol{P}}\left(\varphi_e + C_w\varphi_{wp}\right) : \left[\dot{\boldsymbol{P}} + \boldsymbol{P}\boldsymbol{L}\right]. \tag{8}$$

where we have defined $\varphi_{wp} = \frac{1}{2}|\boldsymbol{W} - \boldsymbol{P}|^2$.

With the explicit form of the conservation laws, and the form of the free energy introduced, we can use a dissipation inequality to derive the kinetic laws governing the evolution of the fields introduced. We write the Second Law of Thermodynamics in the form

$$\int_{\partial\Omega}(\boldsymbol{T}\cdot\hat{\boldsymbol{n}})\cdot\boldsymbol{v}dS + \int_\Omega d\boldsymbol{x}\ \rho\boldsymbol{b} \geq \frac{d}{dt}\int_\Omega d\boldsymbol{x}\ \rho\varphi + \frac{d}{dt}\int_\Omega d\boldsymbol{x}\ \frac{1}{2}\rho|\boldsymbol{v}|^2, \tag{9}$$

so that the power expended by external agencies (applied traction on the outer boundary and the applied body forces) is greater or equal to the rate of change of the free energy plus

kinetic energy. Integrating this relation by parts and using the balance of linear momentum, we write

$$\int_\Omega d\boldsymbol{x}\ \boldsymbol{T} : \boldsymbol{L} - \frac{d}{dt}\int_\Omega d\boldsymbol{x}\ \rho\varphi \geq 0. \tag{10}$$

By explicit substitution of Eq. (5), one finds

$$\begin{aligned}
&\int_\Omega d\boldsymbol{x}\ \boldsymbol{T} : \boldsymbol{L} - \int_\Omega d\boldsymbol{x}\ \rho\left(\frac{\partial\varphi_e}{\partial\boldsymbol{W}} + C_w\frac{\partial\varphi_{wp}}{\partial\boldsymbol{W}}\right) : (-\boldsymbol{W}\boldsymbol{L} + \boldsymbol{\alpha}\times\boldsymbol{V}) \\
&\qquad - \int_\Omega d\boldsymbol{x}\ \left[\varphi_e + C_w\varphi_{wp} + C_\rho\varphi_\rho + C_\rho(\rho-\psi)\right](-\rho\mathrm{Tr}(\boldsymbol{L})) - \\
&\qquad - \int_\Omega d\boldsymbol{x}\ \left[C_{sh}\frac{\delta\Phi_{sh}}{\delta\psi} + C_\rho\rho(\rho-\psi)\right]\dot{\psi} - \int_\Omega d\boldsymbol{x}\ \rho\left[\frac{\partial\varphi_e}{\partial\boldsymbol{P}} + C_w\frac{\partial\varphi_{wp}}{\partial\boldsymbol{P}}\right] : \dot{\boldsymbol{P}} \geq 0
\end{aligned} \tag{11}$$

By using Eq. (8), the last term in the L.H.S. of Eq. (11) can be written as

$$-\int_\Omega d\boldsymbol{x}\ \rho\left[\frac{\partial\varphi_e}{\partial\boldsymbol{P}} + C_w\frac{\partial\varphi_{wp}}{\partial\boldsymbol{P}}\right] : (-\boldsymbol{P}\boldsymbol{L}) - \int_\Omega d\boldsymbol{x}\ \frac{\delta\Phi_{wp}}{\delta\psi}\dot{\psi}$$

This equation can be further rewritten to highlight products of thermodynamics forces and currents as

$$\begin{aligned}
&\int_\Omega d\boldsymbol{x}\ \left[\boldsymbol{T} + \rho\boldsymbol{W}^T\left(\frac{\partial\varphi_e}{\partial\boldsymbol{W}} + C_w\frac{\partial\varphi_{wp}}{\partial\boldsymbol{W}}\right) + \rho a\boldsymbol{I}\right] : \boldsymbol{L} \\
&- \int_\Omega d\boldsymbol{x}\ \rho\left(\frac{\partial\varphi_e}{\partial\boldsymbol{W}} + C_w\frac{\partial\varphi_{wp}}{\partial\boldsymbol{W}}\right) : (\boldsymbol{\alpha}\times\boldsymbol{V}) \\
&+ \int_\Omega d\boldsymbol{x}\ \rho\boldsymbol{P}^T\left(\frac{\partial\varphi_e}{\partial\boldsymbol{P}} + C_w\frac{\partial\varphi_{wp}}{\partial\boldsymbol{P}}\right) : \boldsymbol{L} \\
&- \int_\Omega d\boldsymbol{x}\ \left[C_{sh}\frac{\delta\Phi_{sh}}{\delta\psi} + C_\rho\rho(\rho-\psi) + \frac{\delta\Phi_{wp}}{\delta\psi}\right]\dot{\psi} \geq 0
\end{aligned} \tag{12}$$

where we have defined $a = \varphi_e + C_w\varphi_{wp} + C_\rho\varphi_\rho + C_\rho(\rho-\psi)$.

This expression can be further simplified since the free energy density φ is invariant under rotation. In that case, the antisymmetric (or skew) part

$$\left(\boldsymbol{W}^T\frac{\partial\varphi}{\partial\boldsymbol{W}} + \boldsymbol{P}^T\frac{\partial\varphi}{\partial\boldsymbol{P}}\right)_{\text{skew}} = \boldsymbol{0}.$$

Therefore, of the terms proportional to $\boldsymbol{L}$ in Eq. (12), only those proportional to the symmetric part of velocity gradient $\boldsymbol{D} = (\boldsymbol{L} + \boldsymbol{L}^T)/2$ contribute, and the skew part of $\boldsymbol{L}$ does not appear in the dissipation of the (nonlinear) model, the latter ensuring that the dissipation is invariant under rigid rotations of the body. We combine them into

$$\int_\Omega d\boldsymbol{x}\ \left\{\boldsymbol{T} + \rho\left[\boldsymbol{W}^T\left(\frac{\partial\varphi_e}{\partial\boldsymbol{W}} + C_w\frac{\varphi_{wp}}{\partial\boldsymbol{W}}\right) + \boldsymbol{P}^T\left(\frac{\partial\varphi_e}{\partial\boldsymbol{P}} + C_w\frac{\varphi_{wp}}{\partial\boldsymbol{P}}\right) + a\boldsymbol{I}\right]_{sym}\right\} : \boldsymbol{D} \tag{13}$$

This completes our calculation of the dissipation inequality. One can now identify the reversible parts of the various currents, followed by the introduction of the respective dissipative currents in order to respect the inequality. The symmetric reversible stress follows directly from Eq. (13),

$$\boldsymbol{T}^R = -\rho \left[\boldsymbol{W}^T \left(\frac{\partial \varphi_e}{\partial \boldsymbol{W}} + C_w \frac{\varphi_{wp}}{\partial \boldsymbol{W}} \right) + \boldsymbol{P}^T \left(\frac{\partial \varphi_e}{\partial \boldsymbol{P}} + C_w \frac{\varphi_{wp}}{\partial \boldsymbol{P}} \right) + a\boldsymbol{I} \right]_{sym} \tag{14}$$

Since our formulation applies not only to crystalline phases, but also to other phases with broken symmetries still described by a phase field, we mention that it is possible to introduce a dissipative stress as $\boldsymbol{T}^D = \boldsymbol{\eta} : \boldsymbol{D}$, where $\boldsymbol{\eta}$ is a fourth rank viscosity tensor. The number of independent components of the elastic constant and viscosity tensors depend on the symmetry of the system, and have been enumerated for several important cases [51].

We will restrict our analysis to dissipative defect velocities only. In order to ensure positivity of dissipation, we write

$$\boldsymbol{V} = -\boldsymbol{M}\,\boldsymbol{X} : \left[\rho \left(\frac{\partial \varphi_e}{\partial \boldsymbol{W}} + C_w \frac{\partial \varphi_{wp}}{\partial \boldsymbol{W}} \right)^T \boldsymbol{\alpha} \right] \tag{15}$$

where $\boldsymbol{M}$ is a positive definite mobility tensor, and $\boldsymbol{X}$ is the third rank, Levi-Civita tensor. $\boldsymbol{M}$ cannot be constant in the geometrically nonlinear setting since $\boldsymbol{V}$ has to rotate on a rigid body motion of the body; defining the climb direction as $\boldsymbol{c} = \frac{\boldsymbol{X}:(\boldsymbol{W}^{-1}\boldsymbol{\alpha})}{|\boldsymbol{X}:(\boldsymbol{W}^{-1}\boldsymbol{\alpha})|}$ and $\boldsymbol{M} = \mu_g(\boldsymbol{I} - \boldsymbol{c}\otimes\boldsymbol{c}) + \mu_c \boldsymbol{c}\otimes\boldsymbol{c}$ suffices, where $\mu_g, \mu_c \geq 0$ are glide and climb mobilities, respectively. For $C_w = 0$, it can be shown that the driving force in the above relation corresponds to the exact generalization of the form of the Peach-Köhler force to the fully nonlinear setting [34].

Finally, we identify the reversible and irreversible currents of the phase field ψ. The condition for reversible motion is simply $\dot{\psi} = 0$, that is, advection of the phase field. The dissipative component is chosen to enforce positivity, leading to an order parameter equation,

$$\dot{\psi} = -L \left[C_{sh} \frac{\delta \Phi_{sh}}{\delta \psi} + C_\rho \rho(\rho - \psi) + \frac{\delta \Phi_{wp}}{\delta \psi} \right] \tag{16}$$

where the constant $L > 0$ is the phase field mobility. Importantly, although mass is a conserved quantity, the phase field that describes the broken crystalline symmetry is not. On this particular, our model does differ from implementations of the Phase Crystal model based on density functional theory in which the order parameter is chosen to be the mass density.

In summary, the complete set of equations includes mass (Eq. (1)), momentum (Eq. (2)), and topological charge (Eq. (4) conservation, along with the definition of the dislocation tensor, Eq. (3). The phenomenological currents that follow from the dissipation inequality and the model free energy, Eq. (5), are the stress, Eq. (14), the defect velocity Eq. (15), and the evolution equation for the phase field, Eq. (16).

Before considering the small deformation limit of the model, we outline several qualitative features of the evolution of a defected phase as given by the governing equations. An initially defected configuration will be described by an order parameter field ψ. Topological defects will be located in regions of non zero curl of $\boldsymbol{P}$, with $\boldsymbol{P}$ defined by a point wise oriented triad in reciprocal space, generally not orthonormal, from ψ [19], compared to the same object for the ground state of Φ_{sh}, as explained in the preamble of Sec. II of this paper. For C_w, C_{sh} large and of comparable magnitude, the order parameter will relax quickly (and diffusively) to a local minimum of

$$C_{sh}\Phi_{sh} + \frac{C_w}{2}\int d\boldsymbol{x}\ \rho|\boldsymbol{W}-\boldsymbol{P}|^2$$

relatively independently of the resulting changes induced in the elastic energy φ_e, and in mass density fluctuations. This process will be accompanied by the relaxation of the elastic distortion in phonon lifetime scales, also quickly if the quasistatic elastic limit is invoked. Further evolution will be slow, driven by the Peach-Köhler force in Eq. (15), which is dominated by the elastic stress term $\partial\varphi_e/\partial\boldsymbol{W}$. If the configuration is not initially defected, but subjected to body forces, traction and/or velocity boundary conditions, the solution of the elasticity problem will yield $\boldsymbol{W}$, which will - if C_w and C_{sh} are large - quickly modify ψ. In this case, ψ mediates nonlinear anisotropic elastic response up to the important (microscale) physical phenomenon of homogeneous nucleation of defects.

III. SMALL DEFORMATION LIMIT

In the small deformation or geometrically linear limit, we consider a fixed simply connected reference configuration for the body and assume that the deforming body remains close to this configuration at all times so that all spatial derivatives can be written w.r.t. this fixed reference configuration. As is customary, it is also formally assumed that various distortion measures are 'small' in magnitude. In this case, as mentioned in Sec. II A, the inverse elastic distortion is $\boldsymbol{W} = \boldsymbol{I} - \boldsymbol{U}$ and we treat $\boldsymbol{U}$ as the fundamental measure of

elastic distortion. We note that $\operatorname{curl} \boldsymbol{U} \neq \boldsymbol{0}$ in the presence of defects, when it cannot be written as a gradient of a displacement field. We will also consider the symmetrized elastic distortion $\boldsymbol{\epsilon} = \boldsymbol{U}_{sym}$, $\epsilon_{ij} = (1/2)(U_{ij} + U_{ji})$. Analogously, we define $\boldsymbol{Q} = \boldsymbol{I} - \boldsymbol{P}$.

From Eqs. (3) and (4), the equations defining the dislocation density tensor and defect motion are now

$$\operatorname{curl} \boldsymbol{U} = \operatorname{curl} \boldsymbol{Q} = \boldsymbol{\alpha}, \qquad \boldsymbol{L} = \dot{\boldsymbol{U}} + \boldsymbol{\alpha} \times \boldsymbol{V} \tag{17}$$

where we have neglected the quadratic term $\boldsymbol{U}\boldsymbol{L}$. These equations are the classical equations of plastic motion [22, 44]. Here, $\boldsymbol{L}$ is still the velocity gradient, but now with respect to the fixed reference configuration.

In analogy to Eq. (5) we write the free energy density as

$$\int_\Omega d\boldsymbol{x}\ \varphi(\rho, \boldsymbol{U}, \psi, \boldsymbol{Q}) = \int_\Omega d\boldsymbol{x}\ \varphi_e(\rho, \boldsymbol{U}, \boldsymbol{Q}) + C_{sh}\Phi_{sh}[\psi] + \\ + \frac{C_w}{2}\int_\Omega d\boldsymbol{x}\ |\boldsymbol{U} - \boldsymbol{Q}|^2 + \frac{C_\rho}{2}\int_\Omega d\boldsymbol{x}\ (\rho - \psi)^2. \tag{18}$$

In the small deformation regime, the dissipation inequality is written as

$$\int_\Omega d\boldsymbol{x}\ \boldsymbol{T} : \boldsymbol{L} - \int_\Omega d\boldsymbol{x}\ \dot{\varphi} \geq 0. \tag{19}$$

As in Sec. II, we define

$$\Phi_{uq} = \int_\Omega d\boldsymbol{x}\ \varphi_e(\boldsymbol{U}, \boldsymbol{Q}) + \frac{C_w}{2}\int_\Omega d\boldsymbol{x}\ |\boldsymbol{U} - \boldsymbol{Q}|^2 \tag{20}$$

The second term of Eq. (19) can now be written as

$$\int_\Omega d\boldsymbol{x}\ \dot{\varphi} = \int_\Omega d\boldsymbol{x}\ \frac{\partial \varphi_e}{\partial \boldsymbol{U}} : (\boldsymbol{L} - \boldsymbol{\alpha} \times \boldsymbol{V}) + \int_\Omega d\boldsymbol{x}\ \frac{\delta \Phi_{uq}}{\delta \psi}\dot{\psi} + C_{sh}\int_\Omega d\boldsymbol{x}\ \frac{\delta \Phi_{sh}}{\delta \psi}\dot{\psi}$$

$$+ C_\rho \int_\Omega d\boldsymbol{x}\ \ (\rho - \psi)\,(-\rho \operatorname{Tr}(\boldsymbol{L})) - C_\rho \int_\Omega d\boldsymbol{x}\ (\rho - \psi)\dot{\psi}, \tag{21}$$

where we have used the relation, analogous to Eq.(8),

$$\int_\Omega d\boldsymbol{x}\ \frac{\delta \Phi_{uq}}{\delta \psi}\dot{\psi} = \int_\Omega d\boldsymbol{x}\ \left[\frac{\partial \varphi_e}{\partial \boldsymbol{Q}} + C_w \frac{\partial \varphi_{uq}}{\partial \boldsymbol{Q}}\right] : \dot{\boldsymbol{Q}}. \tag{22}$$

Complete invariance properties under superposed rigid motions is not customarily considered in the geometrically linear theory and hence certain nonlinear terms like $\boldsymbol{Q}\boldsymbol{L}$ in (22) do not appear in Eq. (21).

Since the stress tensor is symmetric, and (infinitesimal) rotational invariance requires that the dependence of φ_e on $\boldsymbol{U}$ be only through the symmetrized distortion $\boldsymbol{\epsilon}$, the dissipation relation Eq. (19) can be written as,

$$\int_\Omega d\boldsymbol{x}\left[\boldsymbol{T}-\frac{\partial\varphi_e}{\partial\boldsymbol{\epsilon}}+C_\rho\rho(\rho-\psi)\boldsymbol{I}\right]:\boldsymbol{L}_{sym}+\int_\Omega d\boldsymbol{x}\,\frac{\partial\varphi_e}{\partial\boldsymbol{\epsilon}}:(\boldsymbol{\alpha}\times\boldsymbol{V})+$$

$$+\int_\Omega\left[-\frac{\delta\Phi_{uq}}{\delta\psi}-C_{sh}\frac{\delta\Phi_{sh}}{\delta\psi}+C_\rho\frac{\Phi_{\rho\psi}}{\delta\psi}\right]\dot{\psi}\geq 0, \tag{23}$$

where we have used the notation

$$\Phi_{\rho\psi}=\frac{1}{2}\int_\Omega d\boldsymbol{x}\,(\rho-\psi)^2.$$

With this form of the dissipation inequality, we can identify the stress and the remaining quantities. The reversible part of the stress is

$$\boldsymbol{T}^R=\frac{\partial\varphi_e}{\partial\boldsymbol{\epsilon}}-C_\rho\rho(\rho-\psi)\boldsymbol{I}, \tag{24}$$

with the dissipative part nominally given by the same expression as in Sec. II. The defect velocity is the standard Peach-Köhler force,

$$\boldsymbol{V}=\boldsymbol{M}\boldsymbol{X}:\left[\left(\frac{\partial\varphi_e}{\partial\boldsymbol{\epsilon}}\right)^T\boldsymbol{\alpha}\right] \tag{25}$$

with $\boldsymbol{M}$ a mobility tensor, positive definite. Finally, as in Sec. II, the reversible part of the evolution of the order parameter is $\dot{\psi}=0$. Adding the dissipative contribution, we arrive at the equation governing the evolution of the phase field,

$$\dot{\psi}=L\left[-C_{sh}\frac{\delta\Phi_{sh}}{\delta\psi}-\frac{\delta\Phi_{uq}}{\delta\psi}+C_\rho\frac{\delta\Phi_{\rho\psi}}{\delta\psi}\right]. \tag{26}$$

The constant $L>0$ is a scalar mobility.

The complete set of equations includes mass and momentum conservation, Eqs. (1) and (2), the simpler kinematic laws valid for small deformations (17), and the phenomenological currents in Eqs. (24), (25), and (26).

A. Example: two dimensional, hexagonal lattice, linear elasticity

In order to illustrate the theory introduced in Secs. II and III, and to compare our results with those of existing treatments, we focus next on the well studied case of a hexagonal lattice

in two dimensions. This case was considered in the original research that introduced the Phase Field Crystal method [1], and has been studied extensively since, including recent analyses of the separation between elastic and plastic time scales [19, 20, 49]. We note, however, that extensions of the phase field crystal method to three dimensions and cubic lattices have also been given [4, 52], and that the example discussed below can be readily extended to three dimensional anisotropic systems as well, including finite deformations. For simplicity, we will also assume a phase of constant density.

The free energy functional appropriate for a two dimensional hexagonal lattice is in dimensionless variables,

$$\Phi_{sh}[\psi] = \int_\Omega d\boldsymbol{x}\ \varphi_{sh} = \int_\Omega d\boldsymbol{x}\ \left[\frac{1}{2}\left[(\nabla^2 + q_0^2)\psi\right]^2 - \frac{\varepsilon}{2}\psi^2 + \frac{g_2}{3}\psi^3 + \frac{1}{4}\psi^4\right], \tag{27}$$

where $q_0 = 1$ (we retain the notation q_0 for ease of presentation), $0 < \varepsilon \ll 1$ is the dimensionless control parameter of the bifurcation between the uniform state $\psi = 0$ and ψ modulated, either along one dimension (a stripe phase) or a hexagonal phase depending on the value of the coupling coefficient g_2. The hexagonal phase is stable when $0 \leq \varepsilon \leq (4/3)g_2^2$. In that case, and assuming $\varepsilon \ll 1$, a slowly varying solution that is locally near a hexagonal phase is

$$\psi(\boldsymbol{x}, t) = \sum_{n=1}^{3} A_n e^{i\boldsymbol{q}_0^n \cdot \boldsymbol{x}} + c.c.$$

where A_n are complex amplitudes that change slowly on the length scale $1/q_0$ ($\mathcal{O}(\varepsilon^{1/2})$), and in time ($\mathcal{O}(\varepsilon)$), and where $\boldsymbol{q}_0^1 = \hat{\boldsymbol{j}}$, $\boldsymbol{q}_0^2 = \frac{\sqrt{3}}{2}\hat{\boldsymbol{i}} - \frac{1}{2}\hat{\boldsymbol{j}}$, $\boldsymbol{q}_0^3 = -\frac{\sqrt{3}}{2}\hat{\boldsymbol{i}} - \frac{1}{2}\hat{\boldsymbol{j}}$, with $\hat{\boldsymbol{i}}$ and $\hat{\boldsymbol{j}}$ the two unit vectors of the Cartesian plane. For any given configuration of ψ the complex amplitudes A_n can be obtained by complex demodulation around $\boldsymbol{q}_0^n$. In steady state, all three amplitudes are equal $|A_n| = A_0$.

In linear elasticity, the response of the hexagonal phase is that of an isotropic material, so that

$$\boldsymbol{T} = \lambda \mathrm{Tr}(\boldsymbol{\epsilon})\boldsymbol{I} + 2\mu\boldsymbol{\epsilon}. \tag{28}$$

For our choice of energy Φ_{sh}, the two Lamé coefficients are $\lambda = \mu = 3A_0^2$ [49].

We first write the kinematic law involving the deformation tensor $\boldsymbol{U}$ and the dislocation density tensor $\boldsymbol{\alpha}$. In two dimensions, one has that $B_j(\boldsymbol{x}) = \alpha_{3j}(\boldsymbol{x})$, where $\boldsymbol{B}$ is the Burgers density vector. As discussed in Sec. II, the tensor $\boldsymbol{P}$ (or $\boldsymbol{Q}$ for small deformation), describes the configurational distortion that is ascribed to the phase field $\psi(\boldsymbol{x}, t)$. In particular,

topological defects of a configuration of ψ are located at the zeros of the complex amplitudes A_n (two amplitudes vanish simultaneously, whereas the third remains finite at the core of a dislocation in the hexagonal lattice). As discussed in detail in Ref. [49], for any contour encircling a defect d at $\boldsymbol{x}_d$ one has,

$$\oint d\theta_n = -2\pi s_n^d$$

where the phase of the wave component n is $\theta_n = \arg A_n$. The topological charge $s_n^d = 0, \pm 1$. Following the definition of Sec. II we write in two dimensions $\boldsymbol{q}_0^1 = \boldsymbol{P}^{-T}\nabla\theta_1$ and $\boldsymbol{q}_0^2 = \boldsymbol{P}^{-T}\nabla\theta_2$, relations that define the configurational distortion tensor $\boldsymbol{P}$. Phase gradients are computed as $\partial_k\theta_n = i\frac{\partial_k|A_n| - e^{-i\theta_n}\partial_k A_n}{|A_n|}$. In the small deformation limit, $\boldsymbol{Q} = \boldsymbol{I} - \boldsymbol{P}$. In three dimensions, the dislocation density tensor then follows as $\operatorname{curl}\boldsymbol{Q} = \boldsymbol{\alpha}$. In two dimensions, one writes the appropriate restriction to the Burgers vector density $\boldsymbol{B}$. The tensor $\boldsymbol{Q}$ as defined satisfies all the requirements in that it is a functional of the phase field only, changes slowly in the scale $1/q_0$ as it depends on the slowly varying phases θ_n, and has the same invariance under rotation as $\boldsymbol{U}$.

In order to complete the determination of the distortion $\boldsymbol{U}$ it is necessary to invoke the equation of elastic equilibrium $\operatorname{div}\boldsymbol{T} = \boldsymbol{0}$. For the hexagonal lattice the elastic problem can be solved by using the constitutive law (28), with the values of the Lamé coefficients that correspond to Eq. (27). In two dimensions and for an isotropic system, the solution can be conveniently expressed in terms of the Airy stress function, as shown in Ref. [19] (in three dimensions the extension is through Kröner's stress function aproach [43]). In the more general case of anisotropic linear elasticity in finite bodies, one generally needs to solve the two equations simultaneously with by now well established numerical techniques [38, 48].

Once the solution of the elastic problem at time t is complete, Eq. (26) determines the evolution of the phase field. The term $\delta\Phi_{sh}/\delta\psi$ is the standard variational derivative of Eq. (27) common to other phase field crystal formulations. Our theory differs from previous studies in the coupling term $\delta\Phi_{uq}/\delta\psi$. As discussed in Sec. II this term, with adequate magnitude of its coupling coefficient C_w, is responsible for the local relaxation of the phase field to enforce that the actual deformation $\boldsymbol{U}$ agrees with the configurational deformation described by ψ. Such a relaxation needs to be fast in the $\mathcal{O}(\epsilon)$ diffusive scale of the phase field, and hence in the scale of topological defect motion through configurational change.

IV. DISCUSSION AND CONCLUSIONS

We have reformulated the Phase Field Crystal model to account for the necessary microscopic independence between the phase field, reflecting the symmetry of the phase, and both mass density and elastic distortion. Although these quantities are related in equilibrium through a macroscopic equation of state, they are independent variables in the free energy, and can be independently varied in evaluating the dissipation functional that expresses the Second Law. We have therefore introduced an independent configurational distortion tensor $\boldsymbol{P}$ which is a pointwise functional of the phase field ψ, but independent of the elastic distortion $\boldsymbol{W}$. It captures the local state of distortion of ψ, including any topological defects. The latter would be located in regions in which $\operatorname{curl} \boldsymbol{P} \neq \boldsymbol{0}$, in analogy with the incompatibility condition of the distortion $\operatorname{curl} \boldsymbol{W} = -\boldsymbol{\alpha}$. In addition, we explicitly include a mass density ρ which is independent of the phase field ψ. These considerations assume that the phase field ψ is a non conserved, broken symmetry variable that reflects the symmetry of the system under study, but that is independent of both mass and distortion.

In order to realistically model defect motion in a crystalline phase, choices need to be made in the magnitude of the coupling terms in the free energy linking the phase variable ψ on the one hand, and $\boldsymbol{W}$ and ρ on the other. Given a material dependent magnitude of the elastic constant tensor $|\boldsymbol{C}|$, we assume that $C_{sh} \sim C_w \gg |\boldsymbol{C}|$. These conditions ensure fast diffusive relaxation of the phase field to accommodate the existing elastic distortion and topology constraints. As discussed in Sec. II, this is accomplished by having the phase field relax to a local minimum of $C_{sh}\Phi_{sh} + \frac{C_w}{2}\int d\boldsymbol{x}\ \rho|\boldsymbol{W} - \boldsymbol{P}|^2$, so that the resulting elastic energy and density fluctuations will then decay in their respective time scales.

Allowing the mass density ρ to be independent of the phase field ψ allows for permeation, the independent motion of mass and lattice. In the case of a monocomponent crystalline solid, for example, this dissipative mode has to be understood as vacancy diffusion. Equations (16) (or Eq. (26) in the small deformation limit) can be interpreted as permeation equations as their right hand sides equal the normal projection of $\boldsymbol{v} - \boldsymbol{v}_\psi$ along the surface of constant ψ, where $\boldsymbol{v}_\psi$ is the local velocity of such a surface. If C_ρ is chosen sufficiently large, then ρ and ψ will locally coincide. However, the ability to separate mass density and phase field is necessary in the treatment of dislocation climb, for example.

The model also naturally incorporates mechanical boundary conditions, either directly

applied to the material velocity field $\boldsymbol{v}$, or traction involving the stress tensor at the boundary $\boldsymbol{T}\hat{\boldsymbol{n}}$. The phase field - also with its own natural boundary conditions - will adjust dynamically in the bulk [49]. Solution procedures for the dislocation mechanics part of the problem at small and finite deformations are detailed in [38, 48]; these are non-standard systems taking into account the nonlinear transport of the dislocation density field and the calculation of nonlinear stress fields of dislocation distributions. The computation of the presented coupled model is the subject of future work.

We close by noting that the formulation developed is applicable not only to crystalline solids, but also to other broken symmetry phases such as colloidal, columnar, and smectic phases.

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Appendix A: Notation and definitions

We use boldface throughout the paper to denote both vectors and rank two (and four) tensors in three dimensional space. Vector and tensor operations are assumed, including differential calculus. All tensor components are expressed w.r.t the basis of a fixed Rectangular Cartesian coordinate system and all partial derivatives are w.r.t the coordinates of this system. We give here a few explicit definitions in terms of vector and tensor components to

avoid possible ambiguity.

If $\boldsymbol{A}$ and $\boldsymbol{B}$ are two tensors, we define $\boldsymbol{A} : \boldsymbol{B} = A_{ij}B_{ij}$. Summation over repeated indices is implied. The cross product with a vector $\boldsymbol{v}$ is given by $(\boldsymbol{A} \times \boldsymbol{v})_{ij} = \epsilon_{jrs}A_{ir}v_s$, where ϵ_{jrs} is the alternating Levi-Civita tensor. Also, in three dimensions, $(\operatorname{curl} \boldsymbol{A})_{ir} = \epsilon_{rjk}\partial_j A_{ik}$.

For kinematics related to the field equations of Burgers' vector conservation and its relation to the evolution of elastic distortion, we refer the interested reader to [45] and Appendix B in [36].