Erratum: Field dislocation mechanics and phase field crystal models [Phys. Rev. B 102, 064109 (2020)]

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(Received 9 June 2025; published 23 June 2025)

DOI: 10.1103/h9cz-2j1b

SECTION II B: BALANCE EQUATIONS

Equation (3) in the original paper should be replaced by

$$\mathrm{curl}\boldsymbol{W} = -\boldsymbol{\alpha}. \tag{E.1}$$

Otherwise, $\boldsymbol{P}$ becomes overspecified by the other kinematic relationships.

SECTION II C: FREE ENERGY, DISSIPATION INEQUALITY, AND GOVERNING EQUATIONS

The analysis of Sec. II C in the original paper starts from an assumed free energy density dependence on field variables $\varphi = \varphi(\rho, \boldsymbol{W}, \psi, \boldsymbol{P})$. However, phase field crystal free energies are based on modifications of the Swift-Hohenberg model (denoted as "sh" in the original paper), which contains a dependence on $\nabla^2\psi$ as well. The Swift-Hohenberg free energy is spatially isotropic, and in the phase field crystal context it leads to a hexagonal lattice in two dimensions, and to a bcc lattice in three dimensions. Lattices of other symmetries can be obtained with more complex combinations of Laplacian operators [1]. Therefore, we replace the free energy dependence assumed in the original paper with $\varphi = \varphi(\rho, \boldsymbol{W}, \psi, \partial_i\psi, \partial_i\partial_j\psi, \boldsymbol{P})$, where $\partial_i = \partial/\partial x_i$ in the current configuration. Hence, the second term on the right-hand side of Eq. (5) in the original paper is instead

$$C_{\mathrm{sh}}\Phi_{\mathrm{sh}}[\psi, \partial_i\psi, \partial_i\partial_j\psi].$$

While this dependence does not cover all phase field crystal models in the literature, the procedure below is relatively simple to describe, and it can be extended to other, more complex cases.

The dissipation inequality (11) contains two additional terms,

$$-C_{\mathrm{sh}}\int_\Omega d\boldsymbol{x}\left[\frac{\partial\varphi_{\mathrm{sh}}}{\partial(\partial_i\psi)}\dot{\overline{(\partial_i\psi)}} + \frac{\partial\varphi_{\mathrm{sh}}}{\partial(\partial_i\partial_j\psi)}\dot{\overline{(\partial_i\partial_j\psi)}}\right], \tag{E.2}$$

where φ_{sh} is the density associated with Φ_{sh}. Its two derivatives depend on the actual functional form of the phase field crystal model used. We also define

$$H_{ij} = \frac{\partial\varphi_{\mathrm{sh}}}{\partial(\partial_i\partial_j\psi)}.$$

The material derivative in the first new term is simple to calculate by using the identity

$$\dot{\overline{\nabla\psi}} = \nabla(\dot{\psi}) - \mathbf{L}^T\nabla\psi, \tag{E.3}$$

where $\boldsymbol{L}$ is the velocity gradients tensor with components $\partial_j v_i$. The second new material derivative is more complicated, although it results straightforwardly from a second application of this identity. Three important observations need to be made, however, in the derivation. First, the requirement that the new free energy φ be invariant under rotation requires a modification to the unnumbered equation between Eqs. (12) and (13) in the original paper. It now reads

$$\left(\boldsymbol{W}^T\frac{\partial\varphi}{\partial\boldsymbol{W}} + \boldsymbol{P}^T\frac{\partial\varphi}{\partial\boldsymbol{P}}\right)_{\mathrm{skew}} + \left(\nabla\psi\otimes\frac{\partial\varphi}{\partial\nabla\psi}\right)_{\mathrm{skew}} + 2((\mathcal{D}^2\psi)\boldsymbol{H})_{\mathrm{skew}} = \mathbf{0}$$

with $(\mathcal{D}^2\psi)_{ij} = \partial_i\partial_j\psi$. This is a necessary condition for rotational invariance of the energy density under superposed rigid body motions.

Second, in order for the dissipation in the theory to be rotationally invariant, the general dependence of Φ_{sh} on $\mathcal{D}^2\psi$ is restricted to satisfy the requirement that the symmetric second-order tensors $\boldsymbol{H}$ and $\mathcal{D}^2\psi$ be coaxial, i.e., they share identical eigenspaces, so that $\boldsymbol{H}\,\mathcal{D}^2\psi$, the product of the two tensors, is symmetric. Most common forms of Φ_{sh} satisfy this requirement, e.g., $\Phi_{\mathrm{sh}} = \Phi_1(\psi, \nabla\psi) + \Phi_2(\mathcal{D}^2\psi)$, with Φ_2 an isotropic scalar-valued function of a symmetric second-order tensor, but more general couplings of $\nabla\psi$ and $\mathcal{D}^2\psi$ are allowed within this restriction.

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Third, the evaluation of $\overline{(\partial_i \partial_j \psi)}^{\cdot}$ requires consideration of gradients of the material spin tensor $\boldsymbol{\Omega} = \boldsymbol{L} - \boldsymbol{D}$ [with $\boldsymbol{D} = (\boldsymbol{L} + \boldsymbol{L}^T)/2$, the rate of deformation/strain rate tensor, which is the symmetric part of $\boldsymbol{L}$]. This gradient is not an independent quantity, but rather it is entirely determined by the strain rate gradient through

$$\partial_k \Omega_{ij} = \partial_j D_{ik} - \partial_i D_{jk}.$$

The dissipation inequality in Eq. (12) of the original paper needs to include the two new terms resulting from Eq. (E.2) [an additional term involving $(\boldsymbol{H}\,\mathcal{D}^2\psi) : \boldsymbol{\Omega}$ arises, but vanishes due to symmetry of $\boldsymbol{H}\,\mathcal{D}^2\psi$]. We do not give them here. Rather, we directly quote the resulting modified reversible stress that replaces Eq. (14) of the original paper (under the assumption that we ignore boundary contributions after integration by parts just as in writing a variational derivative):

$$\begin{aligned}\boldsymbol{T}^R = &-\rho\left[\boldsymbol{W}^T\left(\frac{\partial\varphi_e}{\partial \boldsymbol{W}} + C_w\frac{\varphi_{wp}}{\partial \boldsymbol{W}}\right) + \boldsymbol{P}^T\left(\frac{\partial\varphi_e}{\partial \boldsymbol{P}} + C_w\frac{\varphi_{wp}}{\partial \boldsymbol{P}}\right) + a\boldsymbol{I}\right]_{\text{sym}} \\ &+ C_{\text{sh}}\left(-\nabla\psi\otimes\rho\frac{\partial\varphi_{\text{sh}}}{\partial\nabla\psi} + \nabla\cdot(\rho\boldsymbol{H}\otimes\nabla\psi)\right)_{\text{sym}} - 2C_{\text{sh}}\rho\boldsymbol{H}(\mathcal{D}^2\psi).\end{aligned} \tag{E.4}$$

We note that the last term on the right-hand side of Eq. (E.3) is manifestly nonlinear. Therefore, this new contribution to the dissipation inequality and to the reversible stress would not be present in the limits of small deformation, and, simultaneously, small ψ. This term was not included in Sec. III of the original paper. Additional considerations are necessary in numerical studies in which gradients of the phase of ψ are small (small deformation limit), but, perhaps because of the choice of parameters in φ_{sh}, the amplitude of ψ is of order 1.

SECTION III: SMALL DEFORMATION LIMIT

In going from Eq. (18) to Eq. (21), one term has been dropped. The first line of (21) should read

$$\int_\Omega d\boldsymbol{x}\,\dot{\varphi} = \int_\Omega d\boldsymbol{x}\left[\frac{\partial\varphi_e}{\partial \boldsymbol{U}} + C_w(\boldsymbol{U}-\boldsymbol{Q})\right] : (\boldsymbol{L} - \boldsymbol{\alpha}\times\boldsymbol{V})$$

while the remaining lines are unchanged.

The same term appears in Eq. (23), which now reads

$$\begin{aligned}&\int_\Omega d\boldsymbol{x}\left[\boldsymbol{T} - \frac{\partial\varphi_e}{\partial\boldsymbol{\epsilon}} - C_w(\boldsymbol{U}-\boldsymbol{Q}) + C_\rho\rho(\rho-\psi)\boldsymbol{I}\right] : \boldsymbol{L}_{\text{sym}} + \int_\Omega d\boldsymbol{x}\left(\frac{\partial\varphi_e}{\partial\boldsymbol{\epsilon}} + C_w(\boldsymbol{U}-\boldsymbol{Q})\right) : (\boldsymbol{\alpha}\times\boldsymbol{V}) \\ &+ \int_\Omega\left[-\frac{\delta\Phi_{uq}}{\delta\psi} - C_{\text{sh}}\frac{\delta\Phi_{\text{sh}}}{\delta\psi} + C_\rho\frac{\Phi_{\rho\psi}}{\delta\psi}\right]\dot{\psi} \geqslant 0,\end{aligned}$$

from which two constitutive laws are modified by this extra term. Equation (24) should read

$$\boldsymbol{T}^R = \frac{\partial\varphi_e}{\partial\boldsymbol{\epsilon}} + C_w(\boldsymbol{U}-\boldsymbol{Q})_{\text{sym}} - C_\rho\rho(\rho-\psi)\boldsymbol{I}.$$

Equation (25) is replaced by

$$\boldsymbol{V} = \boldsymbol{M}\boldsymbol{X} : \left[\left(\frac{\partial\varphi_e}{\partial\boldsymbol{\epsilon}} + C_w(\boldsymbol{U}-\boldsymbol{Q})\right)^T\boldsymbol{\alpha}\right].$$

[1] V. Skogvoll, A. Skaugen, and L. Angheluta, Phys. Rev. B **103**, 224107 (2021).