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Phase field modeling with deformation-dependent interface energies

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In the last years, the phase field method has established itself for the simulation of various problem types, especially in the fields of microstructure evolution and phase transformations as well as in fluid dynamics. Concerning the first two cases, usually a constant, deformation-independent, surface energy is considered. In this work, however, deformation-dependent surface elasticity according to [5] will be incorporated into phase field theory. In line with [4], a finite element framework for an Allen-Cahn type phase field model coupled to continuum mechanics is presented, which is solved in a monolithic manner by means of Newton's method. The resulting model also accounts for a spatial evolution of the diffuse interface by a functional of Ginzburg–Landau type. The implemented model is employed in numerical simulations. These will be used to study the behavior of the phase field model.

1 Interface kinematics in continuum mechanics

In order to model two phase systems with interface elasticity, a measurement of deformation within the interface is required. In line with the work in [1], the surface deformation gradient is considered for that purpose. For this, two referential covariant basis vectors $\boldsymbol{G}_\alpha$ (and their contravariant counterparts $\boldsymbol{G}^\alpha$) are introduced as

$$\boldsymbol{G}_\alpha = \frac{\partial \boldsymbol{X}}{\partial \theta^\alpha}, \qquad \left(\boldsymbol{G}_\alpha = \frac{\partial \theta^\alpha}{\partial \boldsymbol{X}} = \frac{\partial \boldsymbol{X}}{\partial \theta_\alpha}\right) \qquad \text{with } \alpha \in \{1,2\} \tag{1}$$

and the spatial basis vectors $\boldsymbol{g}_\alpha$ (and $\boldsymbol{g}^\alpha$) are defined analogously. The surface deformation gradient (a tensor of rank 2) then reads

$$\bar{\boldsymbol{F}} = \boldsymbol{g}_\alpha \otimes \boldsymbol{G}^\alpha. \tag{2}$$

2 Diffuse interface zone

2.1 Elasticity in the interface

The mechanics of the diffuse interface are captured by volume-specific energy

$$\psi_\Gamma = f_{\mathrm{dw}}(p, \nabla p)\, \psi_{\Gamma 0}(\bar{\boldsymbol{F}}), \tag{3}$$

with $\psi_{\Gamma 0}(\bar{\boldsymbol{F}})$ being the underlying area-specific Helmholtz-like energy (in this work: neo Hooke type) and f_{dw}, depending on the phase field parameter p and its gradient. The latter is a smooth approximation of the Dirac delta function, which thus transforms area integrals to volume integrals. From a physics point of view, phase field parameter p represents the relative volume of phase 2.

2.2 Homogenization regarding the bulk phases

Aside from the interface elasticity itself, the material responses of the bulk phases within the diffuse zone need to be taken into account. For that purpose, homogenized, effective energy

$$\psi_{\mathrm{B}} = [1-p]\, \psi_{\mathrm{B}}^{(1)}\left(\boldsymbol{F}^{(1)}, p\right) + p\, \psi_{\mathrm{B}}^{(2)}\left(\boldsymbol{F}^{(2)}, p\right) \tag{4}$$

is employed, cf. [2]. Here, the deformation gradients of the phases $\boldsymbol{F}^{(1)}$, $\boldsymbol{F}^{(2)}$ have been introduced. Following [3], they are assumed as spatially constant and consequently, they can be written as

$$\boldsymbol{F}^{(1)} = [\boldsymbol{F} - \quad p\ [\![\boldsymbol{F}]\!]] \cdot [\boldsymbol{F}_{\mathrm{Bain}}^{(1)}]^{-1}, \qquad \boldsymbol{F}^{(2)} = [\boldsymbol{F} + [1-p]\,[\![\boldsymbol{F}]\!]] \cdot [\boldsymbol{F}_{\mathrm{Bain}}^{(2)}]^{-1}, \tag{5}$$

where $[\![\boldsymbol{F}]\!]$ resembles the jump in $\boldsymbol{F}$ between the bulk phases. It is calculated depending on the choice of a homogenization scheme. For the Taylor-Voigt scheme $[\![\boldsymbol{F}]\!]$ is set to $\boldsymbol{0}$. This does not necessarily fulfill the equilibrium of forces in the interface, though. The other limiting case is the Reuss-Sachs assumption, which determines $[\![\boldsymbol{F}]\!]$ via a local energy minimization. However, this homogenization assumption is not necessarily kinematically compatible. A better approach – fulfilling both conditions – is the rank-1 scheme where the jump in $\boldsymbol{F}$ is calculated from a jump vector $\boldsymbol{a}$ and a normal vector $\boldsymbol{N}$, which are in turn again obtained via a local minimization. Clearly this option is motivated by the Hadamard jump condition. However, this work sticks to the Taylor-Voigt assumption.

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2.3 Variational framework

The total energy of the system consists of the volume and surface contributions ψ_{B} and ψ_{Γ}, as well as contributions due to external work. Since interfaces are usually linked to dissipation, an additional dissipation term $\phi(\dot{p})$ of Ginzburg–Landau type is also employed, depending on the rate of p. Based on these definitions, rate (or incremental) energy

$$\begin{aligned}\Delta\mathcal{E} = &\int_{\mathcal{B}_0} \psi_{\mathrm{B}}(t_{n+1})\,\mathrm{d}V - \int_{\mathcal{B}_0} \psi_{\mathrm{B}}(t_n)\,\mathrm{d}V + \int_{\mathcal{B}_0} \psi_{\Gamma}(t_{n+1})\,\mathrm{d}V - \int_{\mathcal{B}_0} \psi_{\Gamma}(t_n)\,\mathrm{d}V \\ &- W_{\mathrm{ext}}(t_{n+1}) + W_{\mathrm{ext}}(t_n) + \int_{\mathcal{B}_0} \Delta t\,\phi(\dot{p})\,\mathrm{d}V\end{aligned} \tag{6}$$

is considered, cf. [4]. The motion $\boldsymbol{\varphi}$ and the phase field parameter p can then be obtained via $\{\boldsymbol{\varphi}, p\} = \arg\inf(\Delta\mathcal{E})$ as minimization arguments. For the sake of completeness it should be mentioned, that additional penalty terms were utilized in order to enforce $0 \le p \le 1$.

3 Numerical example

The model was discretized and incorporated into a FE algorithm, resulting in a fully coupled model which is solved monolithically. As a numerical experiment a hollow sphere, that is subjected to homogeneously distributed radial displacements on the outer shell, is considered, cf. Figure 1. The chosen example allows for the use of symmetries in order to reduce the model to 1d. While for smaller values of u_{pre} the interface energy contribution dominates, the bulk energy becomes the major driving force for larger deformations.

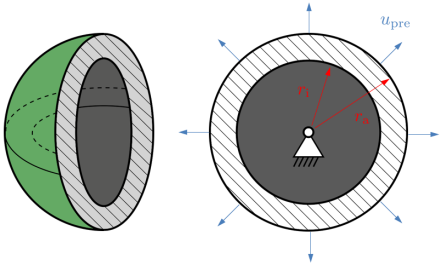

Fig. 1: Illustration of a hollow sphere, cut open for the sake of better understanding. The inner void is represented by a phase with significantly reduced elastic stiffness (factor 1e+2).

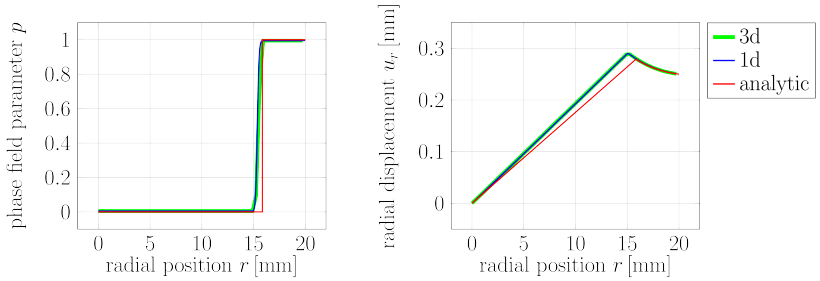

Fig. 2: Comparison of phase field parameter p and radial displacements u_{r} for the 3d simulation, 1d simulation and analytic calulations.

For this example a full 3d framework is compared to the symmetry using 1d algorithm as well as to an analytic solution. The results for $u_{\mathrm{pre}} = 0.25\,\mathrm{mm}$ after a relaxation period are shown in Figure 2. The curves for 1d and 3d are almost identical, ensuring that the reduced model works just as well as the full 3d one. The interface position of these two simulations differs slightly from the analytic results. Here it needs to be stated that the analytic results was calculated using a sharp interface. Furthermore, the choice of the homogenization scheme may have additionally influenced the result. However, the numerically obtained results fit the analytic ones quite well.

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