Documentation
PRISMS-PF: Equilibrium Shape for a Misfitting Precipitate

Overview:

This tool simulates the shape of a two-dimensional precipitate based on anisotropic interfacial energy, anisotropic misfit strain, and the elastic properties (Young's modulus and Poisson's ratio) of the precipitate and matrix material. This is a black-box simulation tool that only requires users to input the materials parameters for the simulation; simulation conditions are specified within the code. In the PRISMS-PF Misfit tool, the simulation begins with a round precipitate, which is then evolved using Allen-Cahn dynamics until the specified tolerance is reached. The tool utilizes the PRISMS-PF open-source phase-field modelling framework; documentation of PRISMS-PF is available at https://prisms-center.github.io/phaseField/.

Inputs:

The inputs for the simulation are given in the table below. The 1 and 2 notations utilize the standard notation for directions. In these simulations, the x-direction and y-direction can be taken to be directions 1 and 2, respectively.

The misfit strain is taken from the stress-free transformation strain tensor (SFTS), $\boldsymbol{\epsilon}$, where

$$\boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_{1,1} & \epsilon_{1,2} & \epsilon_{1,n} \\ \epsilon_{2,1} & \epsilon_{2,2} & \epsilon_{2,n} \\ \epsilon_{3,1} & \epsilon_{3,2} & \epsilon_{3,n} \end{pmatrix}.$$

Other orientations may be simulated using the appropriate tensor rotation.

Input	**Description**	**Minimum**	**Maximum**
Interfacial Energy			
(1,1) component (mJ/m^2)	The energy of the precipitate/matrix interface along the x-axis	4	35
(2,2) component (mJ/m^2)	The energy of the precipitate/matrix interface along the y-axis	4	35
Misfit Strain			
(1,1) Component	The (1,1) component of the misfit strain tensor	-0.1	0.1
(2,2) Component		-0.1	0.1
(1,2) Component		-0.1	0.1

(2,1) Component		-0.1	0.1
Elastic Constants (Matrix)			
Young's Modulus (GPa)		30	100
Poisson's Ratio		0.25	0.35
Elastic Constants (Precipitate)			
Young's Modulus (GPa)		30	100
Poisson's Ratio		0.25	0.35

Modes:

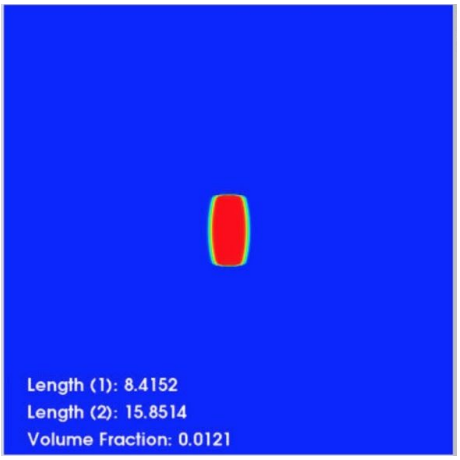
The simulation tool can be run in two modes: low fidelity (Lo-Fi) and high-fidelity (Hi-Fi). The completion of the simulation is set based on the specified **tolerance**, which measures the change in the integrated nondimensionalized free energy over the course of 50,000 time steps. The tolerance values for Lo-Fi and Hi-Fi modes are 10^{-3} and 10^{-6}, respectively. The larger tolerance for the Lo-Fi mode causes the simulation to run faster, but at lower accuracy, compared to the Hi-Fi mode. Hi-Fi is the default run condition, but Lo-Fi mode may be utilized for initial investigation of the parameter space or for educational modules where *only* qualitative shapes are needed. After selecting the optimal set of materials parameters, it is recommended that users repeat these simulations in Hi-Fi mode.

Running a Simulation

The run time may be instantaneous, or it may take several hours. Instantaneous results may be provided from cached results of prior simulations with the same input conditions and Lo-Fi/Hi-Fi mode. Otherwise, the run time is dependent on the strength of the anisotropy, particularly interfacial energy anisotropy, and Lo-Fi/Hi-Fi mode.

Results

The simulation outputs an image of the precipitate morphology, such as the one shown below.



The colors indicate the value of the order parameter at each point (the matrix and precipitate are blue and red, respectively). The gradual change between the two phases (indicated by the other colors) is due to the diffuse interface required for the phase-field model; the width of this diffuse interface may be non-uniform due to anisotropy. The size of the precipitate in the x- and y-directions are represented by lengths (1) and (2), respectively.

Supplementary Material

A corresponding educational module has been developed and is shared on nanoHUB:

> Susan P Gentry, Stephen DeWitt, Mingwei Zhang (2019), "Simulating Precipitate Morphology using a Phase Field Model," https://nanohub.org/resources/31734.