My research has focused on the epitaxial growth of thin films, martensitic microstructure, finite element superconvergence, and stress-driven interface dynamics.

1. Epitaxial Growth of Thin Films

Epitaxial growth is a widely used technique to grow thin solid films by depositing atoms or molecules onto an existing layer of material. It has applications in many modern technologies. Microscopic processes in epitaxial growth include the deposition of atoms from the gas phase onto a film surface, desorption of adatoms (adsorbed atoms) from such surface into the gas phase, surface diffusion of adatoms, nucleation of adatom islands, attachment and detachment of adatoms to and from atomic steps or island boundaries, and island coalescence. These processes are often far from equilibrium, and span several decades of spatial and temporal scales.

1.1. Analysis and improvement of island dynamics models.

Burton, Cabrera, and Frank (Phil. Trans. Roy. Soc. Lond. Ser. A, 243:299–358, 1951) developed the first detailed description for epitaxial growth: the adatom density solves a diffusion equation with an equilibrium boundary condition, and step edges move with a velocity determined from the two-sided diffusive flux to the boundary. This BCF model has been widely used for many decades. However, its assumption on equilibrium steps is invalid in many experimental situations in which the growth of thin films is far from equilibrium. Only very recently, Caflisch et al (Phys. Rev. E, 59:6879–6887, 1999) have developed a kinetic step model to include the missing kinetics. But this new model is too complicated for analysis and simulation. And the question arises: what are the right boundary conditions and velocity law in a simple BCF-like model that includes the step kinetics?

In our joint work [11], Caflisch and I have answered this question. Besides various kinds of results, we used a method of asymptotic expansion to eliminate, up to the leading order, the edge-adatom density and kink density in the complicated kinetic step model. We further applied a multiscale analysis to derive rigorously a new set of boundary conditions that is a kinetic version of the Gibbs-Thomson relation and normal velocity law that includes the “surface diffusion” along step edges. Various forms of such boundary conditions and velocity law exist in literature. However, to the best of our knowledge, this derivation is the first that is based on kinetics rather than thermodynamics.

To validate this new set of boundary conditions and velocity law, in the joint work [17], we studied the morphological stability of a single, circular, epitaxially growing adatom island whose properties are often experimentally accessible. Unlike a flat interface in many materials science problems, there is no kinetic steady-state solution with a constant normal velocity for a circular object in a diffusional field. However, we developed a framework for the rigorous analysis of stability for a circular island with radially symmetric adatom distribution with respect to perturbation in both radial and angular directions. Among many interesting stability results, we found that the Bales-Zangwill instability (Phys. Rev. B, 41:9, 5500–5508, 1990) for a straight atomic step due to the kinetic asymmetry disappears for a circular island.

1.2. An adaptive finite element method for island dynamics.

In [16], my collaborators and I developed an adaptive finite element method for the numerical simulation of island dynamics in epitaxial growth, using a BCF type island dynamics model with the new set of boundary conditions and normal velocity. Most of the current simulations of the island dynamics use the level-set formulation with the finite difference discretization. To include in the velocity law the one-dimensional “surface diffusion”—the second-order tangential derivative of the curvature, one needs to discretize fourth-order derivatives on a Cartesian grid that is cut by curved island boundaries. This can be very complicated and inefficient. The approach developed in our work [15], however, lowers the order of the derivatives by using a variational formulation, and only uses linear finite elements to discretize both the adatom diffusion and boundary evolution. Numerical tests on pure geometrical motion, mass balance, and the
stability of a growing circular island demonstrate that our method is stable, efficient, and accurate enough to simulate the growing of epitaxial islands over a sufficiently long time period.

1.3. Analysis of continuum models for epitaxial growth. For the past decade, there have been considerable efforts made in the physics community to study continuum models of epitaxial growth in terms of scaling laws. When stochastic effects are negligible, such models are the initial-boundary-value problems of diffusion equations for the film height profile. In [14], Liu and I studied two continuum growth equation models, with or without slope selection, that are gradient flows of the free energy functionals of the (scaled) film height profile $h = h(x,t)$

$$E_1(h) = \int \left[ \frac{1}{4} (|\nabla h|^2 - 1)^2 + \frac{\varepsilon}{2} |\Delta h|^2 \right] dx,$$

$$E_2(h) = \int \left[ -\frac{1}{2} \ln (1 + |\nabla h|^2) + \frac{\varepsilon}{2} |\Delta h|^2 \right] dx,$$

respectively, where $\varepsilon > 0$ is a small parameter. We proved the well-posedness of the initial-boundary value problem for each of these growth equations. We also demonstrated by weakly nonlinear analysis and numerical simulation a morphological instability in the rough-smooth-rough pattern that agrees with experiments reported by Gyure et al (Phys. Rev. Lett., 81:4931–4934, 1998). Finally, we developed a Galerkin spectral method for numerically solving these equations. This numerical method has been improved in [23] to treat more general growth equations.

In [18], Liu and I continue to study the growth equation without the slope selection, focusing on the underlying coarsening dynamics and energetics. We first prove for large time $t$ that the interface width—the standard deviation of the height profile—is bounded above by $O(t^{1/2})$, the averaged gradient is bounded above by $O(t^{1/4})$, and the averaged energy is bounded below by $O(- \log t)$. We then consider a small coefficient $\varepsilon^2$ of $|\Delta h|^2$ with $\varepsilon = 1/L$ and $L$ the linear size of the underlying system, and study the energy asymptotics in the large system limit $\varepsilon \to 0$. We show that global minimizers of the free energy exist for each $\varepsilon > 0$, the $L^2$-norm of the gradient of any global minimizer scales as $O(1/\varepsilon)$, and the global minimum energy scales as $O(\log \varepsilon)$. The existence of global energy minimizers and a scaling argument are used to construct a sequence of equilibrium solutions with different wavelength. Finally, we apply our minimum energy estimates to derive bounds in terms of the linear system size $L$ for the saturation interface width and the corresponding saturation time.

1.4. The sine-Gordon relaxation in epitaxial growth. Following the work by Chui and Weeks (Phys. Rev. Lett., 40:733–736, 1978) on the roughening transition in epitaxial growth, my collaborator and I have recently studied a continuum sine-Gordon model that is determined by the free energy [22]

$$E(h) = \int \left[ G(\nabla h, \nabla^2 h) + \lambda \cos(2\pi h) \right] dx,$$

where $h$ is the film height profile, $G(\nabla h, \nabla^2 h)$ a usual smoothing term that can be non-quadratic to include various microscopic effects, and $\lambda$ a parameter that depends on temperature. As the first step, we choose $G(\nabla h, \nabla^2) = (1/2)|\nabla h|^2$ or $|\nabla h|$ in (1). We study the partial differential equation aspects of the resulting gradient system without noise. We also develop numerical methods for both of the conservative and non-conservative relaxation dynamics.

I will continue to study continuum models for epitaxial growth, trying to understand the coarsening phenomena, reduced dynamics, and small surface diffusion limit. I will also improve the sine-Gordon relaxation model to include more general relaxation mechanisms such as the surface diffusion and to include the stochastic effect. Finally, I will develop phase field models for electro-migration in step-flow epitaxial growth to seek the possibility of evolving current-induced unstable surfaces into well-organized nanostructures, and to show the effectiveness of possibly negative kinetic rates.

2. Martensitic Microstructure

A martensitic crystal such as a shape-memory alloy has a symmetric lattice structure known as austenite that is stable at a high temperature and several less symmetric lattice structures known
as martensite or martensitic variants that are equally stable at a low temperature. Upon changing
temperature or applying stress, such a crystal undergoes a reversible phase transformation between the
austenite and martensite or between the martensitic variants. The experimentally measurable lattice
changes from the austenite to martensitic variants are described by transformation matrices $U_1, \ldots, U_N$
with $N$ the number of variants. During a martensitic transformation, a fine-scale mixture of coherent
martensitic variants such as a twin or laminate appears. This is martensitic microstructure. It enables
a martensitic crystal to recover its strain and change its shape.

In the geometrically nonlinear continuum theory, the martensitic microstructure is modeled as to
minimize a free energy

$$E(y) := \int_{\Omega} \phi(\nabla y(x)) \, dx$$

among all admissible deformations $y : \Omega \to \mathbb{R}^3$, where the reference configuration $\Omega \subset \mathbb{R}^3$ is the austenite
of the underlying crystal, $\phi : \mathbb{R}^{3 \times 3} \to \mathbb{R}$ a rotationally invariant energy density, and $\mathbb{R}^{3 \times 3}$ the set of all
real $3 \times 3$ matrices. The energy density $\phi$ is assumed to attain its minimum (scaled to be 0) exactly on
$\text{SO}(3)U_1 \cup \cdots \cup \text{SO}(3)U_N$ representing the martensitic variants, where $\text{SO}(3)$ is the set of all $3 \times 3$ proper
rotation matrices. Due to the coexistence of these multiple energy wells, the total energy (2) does not
in general have an admissible minimizer. Energy-minimizing sequences of deformations with oscillatory
gradients, however, generate Young measures that give the distribution of energy-minimizing gradients.

A commonly observed martensitic laminate is locally a continuous deformation whose gradient takes
constant values $A \in \text{SO}(3)U_i$ on one side and $B \in \text{SO}(3)U_j$ on the other side of a planar interface for
some $i, j$ with $1 \leq i, j \leq N$ and $i \neq j$, where $A$ and $B$ are rank-one connected as

$$A - B = a \otimes n$$

for some $a, n \in \mathbb{R}^3$ depending on $i, j$ with $n$ the interface normal. To model a fine-scale laminate (or
laminated microstructure) composed of the gradients $A$ and $B$ with volume fractions $\lambda$ and $1 - \lambda$, one
minimizes the energy (2) among all deformations $y$ that satisfy the boundary condition $y(x) = F_\lambda x$
(x $\in \partial\Omega$) with

$$F_\lambda = \lambda A + (1 - \lambda)B.$$  

(4)

For both the two-well and three-well problems, Ball and James (Phil. Trans. R. Soc. Lond. A, 338:389–
450, 1992) proved that such boundary condition uniquely determines the Young measures generated by
any energy-minimizing sequence of deformations.

2.1. Finite element analysis of a laminated martensitic microstructure. In the mid 1990’s,
finite element computations were performed extensively to validate analytical results on martensitic
microstructure. Luskin (Numer. Math., 75:201–221, 1997) gave an analysis for the conforming finite
element approximation of a laminated microstructure for a two-well ($N = 2$) problem. In [4–6], Luskin
and I generalized this analysis to both conforming and nonconforming finite element approximations of
a laminated microstructure with constant or varying volume fractions governed by both the two-well
and three-well problems.

2.2. Uniqueness of a laminated microstructure. For a multi-well problem with $N \geq 4$, are the
Young measures generated by energy-minimizing sequences of deformations still uniquely determined by
the boundary condition that is consistent with a laminated microstructure? In this setting, the energy
density $\phi$ attains its minimum on the $N$ energy wells, but the boundary data $F_\lambda$ defined by (4) only
involves two variants. The difficulty in showing the uniqueness therefore lies in the exclusion, sorely by
the boundary condition, of all the variants other than those two.

In 1999, Bhattacharya, Luskin, and I [9] proved such uniqueness and obtained stability estimates for
a laminated microstructure for a six-well problem. Our main ideas were to study the strong convergence
of both the sequence of gradients and that of cofactors of gradients in the direction $w \in \mathbb{R}^3$ tangential
to the twin planes defined by the rank-one connections (3) and by

$$\text{Cof} A - \text{Cof} B = -(\det A)A^{-1}a \otimes B^{-T}n$$

which follows from (3), respectively, and choose suitable such vectors $w$. 3

2.3. Microstructure with general homogeneous boundary data. In [10], I studied multi-well energy-minimization problems with general homogeneous boundary data for a large class of martensitic transformations that either are themselves or can be essentially reduced to two-dimensional. Such problems often lack the uniqueness of Young measure solutions, and are thus significantly different from those modeling a simply laminated microstructure. Based on the observation that the underlying microstructures result essentially from in-plane deformations, I was able to develop a stability theory for such microstructures. In particular, I proved that the macroscopic deformation, i.e., the gradient of the weak limit of an energy-minimizing sequence, is unique and the same as the boundary data. I also proved that the projection \( \pi : \mathbb{R}^{3\times 3} \to SO(3)U_1 \cup \ldots \cup SO(3)U_N \), which has been frequently used, is well-defined and Borel measurable.

Parallel to the theory, in [12], I carried out the numerical analysis for such energy-minimization problems. For the finite element approximation of a laminated microstructure of order \( q \geq 1 \) with quasi-uniform meshes, I obtained an \( O(h^{1/(q+1)}) \) energy bound, where \( h \) is the mesh size.

2.4. Numerical modeling of the Chu-James microstructure. In their biaxial loading experiments on the shape-memory alloy Cu-Al-Ni single crystals, Chu and James discovered a needle-like martensitic microstructure near an interface between twinned martensitic layers and a pure variant of martensite (cf. C. Chu, Ph.D. thesis, University of Minnesota, 1993). The layers of one variant form long, branched, and bent needles ending at the nearly flat interface while the others are compatible with a homogeneous state at the interface. In my thesis [20] and the joint work [7], we constructed a continuum model for the Chu-James needle-like microstructure. Our analysis using such a model predicted the orientation misfit agreeing with the experiment almost exactly. We developed a finite element method and optimization algorithm for the simulation of the microstructure. Our large-scale computations captured many features of the microstructure, such as the branching and bent needles. Moreover, we also discovered computationally a complex microstructure with multiple length scales that turned to be experimentally observed.

Currently, I am developing multi-scale models and hybrid numerical techniques to study different physical effects, such as the kinetics, anisotropic interfacial energy, and stresses, in the formation and evolution of martensitic microstructure.

3. Finite Element Superconvergence

Let \( V \) be a function space and \( u \in V \) the solution of a second-order, elliptic, boundary-value problem. Let \( V_h \) be a finite element space containing all piecewise polynomials of degree up to \( k \geq 0 \) and \( u_h \in V_h \) the finite element solution, where \( h \) is the mesh size. Typically,

\[
\| u - u_h \| \leq Ch^{k+1} \quad \text{and} \quad \| \nabla (u - u_h) \| \leq Ch^k,
\]

where \( \| \cdot \| \) is the \( L^2 \) or \( L^\infty \) norm and \( C = C(u) > 0 \) a constant independent of \( h \). These estimates are optimal. However, practical computations often show higher order approximations

\[
| (u - u_h)(z_h) | = O \left( h^{k+2} \right) \quad \text{or} \quad | \nabla (u - u_h)(z_h) | = O \left( h^{k+1} \right)
\]

on special sets of discrete points \( z_h \) such as element centers, where \( \nabla \) is an averaged gradient. This is \textit{superconvergence}. Its mathematical study began in the early 1970’s.

3.1. Superconvergence for conforming simplicial finite elements. There are three key steps in a traditional approach to studying the superconvergence for conforming (defined by \( V_h \subset V \)) simplicial finite elements (triangles and tetrahedrons). First, identify superconvergence points for the Lagrange interpolant \( L_h \). Second, establish higher order, weak energy estimates such as

\[
| a(u - L_h u, v_h) | \leq Ch^{k+1} \| \nabla v_h \|_{L^2} \quad \forall v_h \in V_h,
\]

(5)
where \( a : V \times V \to \mathbb{R} \) is the underlying bilinear form. Third, replace \( v_h \) in (5) by the finite element Green’s function and estimate its norm. The first and third steps work for general \( k \geq 1 \). In the 1980’s, the key estimate (5) was obtained for \( k = 1, 2 \) by the cancellation of quantities contributed from neighboring elements to integrals over the common element boundaries.

Can one still use the traditional approach to obtain the superconvergence for conforming simplicial finite elements of higher order \( k \geq 3 \)? In 1990, I constructed counterexamples to answer this question negatively [1]: for the cubic triangular element (\( k = 3 \)), the estimate (5) no longer holds true, and the Lagrange interpolation points and the superconvergence points for the finite element solution are not identical! The key observation here is that there is an interior nodal point for the cubic element. Consequently, a bubble function \( v_h \in V_h \) that vanishes on all element edges can be constructed to make it impossible for the technique of cancellation to work.

Questioning the generality of the traditional approach to superconvergence, this work [1] has received much attention. (For example, it was stated to be “important” in L. Wahlbin’s monograph, *Superconvergence in Galerkin Finite Element Methods*, Springer-Verlag, 1995. In the description of the workshop *Superconvergence in Finite Element Methods*, Berkeley, 2000, the organizers wrote: “However, in 1990 it was found that the natural analogue of this [i.e., the Lagrange interpolation] is false for cubic elements”, see http://www.msri.org/activities/programs/9900/fem/superconv/.) Babuška et al (Numer. Methods for PDEs, 12:347–392, 1996) reported numerical experiments confirming some of the results in [1]. Schatz, Sloan, and Wahlbin (SIAM J. Numer. Anal., 33:501–521, 1996) developed a new approach to obtain more (but still not the most) general results. Recently, in [15], I have generalized my work [1] to simplicial finite elements of any order \( k \) in any space dimension \( d \geq 2 \) with \( k \geq d + 1 \). The last inequality means exactly the existence of an interior nodal point of a simplicial element.

### 3.2. Superconvergence for nonconforming finite elements.

The mathematical justification of the superconvergence for nonconforming finite elements (defined by \( V_h \not\subset V \)) had been open for quite a few years. In [19], I solved this open problem for the Wilson nonconforming finite element in a special setting. The main idea in the analysis was to decompose the underlying nonconforming finite element space \( V_h \) into the sum of a conforming finite element space and a set of nonconforming, correction functions. In [2], Chen and I further applied an improved version of the decomposition technique to study the Wilson nonconforming element in a general setting. Besides superconvergence estimates, we also obtained the solution expansion that can be used for many post-processing methods, such as the Richardson extrapolation and defect correction, and lower bounds on the solution error in terms of negative norms. All of these results indicate that the Wilson element is asymptotically not better than the conforming bilinear finite element.

The techniques developed in these works [2, 19] are fairly general. In my joint work [3], for instance, we applied these techniques to obtain the superconvergence for the rotated trilinear elements, a class of nonconforming elements that have been applied to the Stokes problem modeling incompressible fluids and nonconvex variational problems modeling crystalline microstructure.

### 3.3. Superconvergence patch recovery technique.


At present, I am concerned with the following three issues on the finite element superconvergence: (a) the relaxation of severe mesh restrictions usually needed for superconvergence; (b) superconvergence for nonconforming finite elements for fourth-order problems with application to plates; and (c) superconvergence up to boundaries with application to interface motion.

### 4. Stress-Driven Interface Dynamics

I have been recently developing a new research area on stress-driven interface dynamics that is important in materials science. Examples of interest include the interface motion in stress-driven martensitic
phase transformations, the evolution of microstructure in an elastically stressed solid undergoing a diffusional phase transition, the Asalo-Tiller-Grinfeld instability in the evolution of a traction-free surface bounding an elastic material, and the stress effect in the epitaxial growth of thin films that is responsible for the formation of nanoscale structures such as quantum dots. My objectives are to: (a) use mathematical tools to derive and analyze rigorously some of the existing models; (b) develop hybrid, multi-scale numerical methods for large-scale computations.

My preliminary work along this line includes [13, 24] on efficient numerical methods for elasticity problems with curved interfaces and [21] on the morphological evolution of solid thin films with an array of periodically distributed dipoles of edge dislocations along interfaces of different layers.

References—My Publications

Published Journal Articles


Articles Submitted for Publication


Other Articles

[22] Bo Li and Bing Song. The sine-gordon relaxation in epitaxial growth. 2004 (work in progress).