Research Interaction Team Plan

Team name. Modeling, analysis, and computation of interfaces in materials science.

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Research focus. The understanding of surfaces and phase boundaries in materials science is a rich source of mathematical problems. Progress requires an integrated approach including modeling, analysis, and computation. Initial efforts will focus on the following problem areas:

(1) the dynamic development of atomic-scale steps on crystal surfaces;
(2) complex microstructures arising through energy minimization; and
(3) stress-driven morphological instabilities in solid thin films.

Analytical techniques will include modern methods in nonlinear dynamics, PDEs, and the calculus of variations. Methods of numerical computation to be investigated will involve adaptive schemes and multiscale techniques.

We aim to develop and capitalize on existing collaborations with physicists and materials scientists around the campus (such as the MRSEC center in Physics, IPST, and the Materials Sci. Dept.) and in the region (such as NIST).

Graduate prerequisites. Introductory PDEs (MATH 462) and numerical computation (AMSC 460 or 466). Concurrent enrollment in advanced PDEs (MATH 673-674) and numerical analysis and/or scientific computing (AMSC 666 and/or 660). Knowledge of continuum mechanics and elasticity will be useful but not required.

Undergraduate prerequisites. Advanced calculus (MATH 241) and differential equations (MATH 246). Concurrent enrollment in scientific computing (MATH 460).

Graduate program. Exposure to the fundamental ideas in the field will be gained through reading seminal papers and making presentations in team meetings. Students will be encouraged to develop interdisciplinary involvement by attending some physics and/or materials science seminars, and giving a 5 minute report in a team meeting. As opportunity allows, graduate students will serve as consultants on undergraduate projects.

Undergraduate program. Research opportunities include numerical simulation and experimentation using Matlab for one-dimensional models of: the dynamics of steps on crystal surfaces; surface evolution of semiconductor thin films; and microstructure evolution by nonconvex energy minimization.

Work schedule.

Phase 1. Faculty give seminars or short courses introducing the main subjects.
Phase 2. Graduates read major papers and report progress to the team for discussion. Undergraduates begin computational experiments.
Phase 3. Project-oriented small groups work independently for discussion and to solve problems.
Phase 4. Graduates make presentations in seminars. Where appropriate, students disseminate results in forums in the department, campus-wide, and on the web.

An organizational meeting will be held in early September.