TEMPLE UNIVERSITY
Department of Mathematics

Applied Mathematics and Scientific Computing Seminar

Room 617 Wachman Hall

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Understanding Material Behavior via Multiscale Mathematical Analyses and Numerical Simulations

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Abstract.

In this talk we will discuss two problems of high technological relevance and present two different multiscale strategies to tackle them. The first of them discusses the modeling of large plastic deformations in metallic systems, which is essential in many manufacturing processes, in permanent fixtures or as energy absorption mechanisms. The length and time scale involved in these processes is not amenable to lower scale models such as atomistic calculations or dislocation dynamic simulations, and continuum models and simulations present the only viable solution. However, the basic kinematic assumptions underlying these continuum models are not completely understood and many open problems still remain unresolved. In this talk we will unveil some of these issues via multiscale kinematic analysis of elastoplastic deformations. The second problem that we will discuss is concerned with the crystallization of Germanium from amorphous thin films - an important process for memory devices based on phase change materials-. Similarly to the first example, molecular dynamic simulations are prohibitive to understand the interplay between nucleation and growth in the crystallization process and continuous phase field models represent an attractive solution. In this talk we will present a novel parametrization strategy of the phase field equations from atomistic calculations that allow for an exact representation of the essential energetic and kinetics features of amorphous-crystalline interfaces. This multiscale approach will then be used to study Ge-nanocrystallization with high physical fidelity and deliver universal laws that characterize this process for a wide range of nucleation rates.