Computational Nano-Engineering for Patterned Magnetic Nanostructures

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Abstract – 0085569 – Gao, Nix, Cho, Clemens – Stanford University

Computational nano-engineering is an emerging field of research aimed at developing nanoscale modeling and simulation methods to enable and accelerate the design and development of functional nanometer-scale devices and systems. Just as microfabrication has led to microelectronics revolution in the 20th century, nano-precision engineering will be a key to the nanotechnology revolution in the 21st century. A major challenge in this technology is to fabricate patterned nanostructures. The objective of the proposed research is to develop multiscale modeling and simulation methods for nanopatterning. As a prototype example with comprehensive industrial impact, we will focus our efforts on nanopatterning of magnetic nanostructures for high-density information storage device applications where the control of grain size distribution is becoming increasingly important, and the drive for decreased media noise and increased storage density is pushing the grain size below the 10 nm regime.

We propose a systematic study of the mechanisms that control the grain size and grain size distribution in magnetic thin films. We will use continuum theories to model the length scales determined by competing mechanisms of epitaxy, surface stress, surface energy, strain energy, compositional free energy and quantum energy. We will develop kinetic Monte Carlo and quantum simulations to simulate nanoscale self-organization for creating magnetic thin film media with ultra-fine grain sizes and ultra-narrow grain size distributions. The simulation tools will allow us to quantitatively investigate nanofabrication processes, and in particular, to predict the grain size and grain size distribution in magnetic nanostructures.

The proposed project will have immediate impact on the magnetic information storage nanotechnology by providing industry with the first theoretical tool to analyze nanofabrication processes based on the state-of-the-art knowledge of nanoscale modeling and simulation. This project will allow engineers to reduce or eliminate costly and slow processes of developing new nanostructured materials. Through the proposed research, we will develop the framework of computational nanopatterning technology which will benefit the whole spectrum of current nanotechnology challenges. This project will lead to better understanding of the basic mechanisms that control the structuring of materials at the nanometer scale. The Kinetic Monte-Carlo simulation and quantum simulation methods developed under this project will have far-reaching significance for the design and manufacturing of nanodevices.