

MAR06-2005-000966

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

Inverse Design of Surface-Based Magnetic Nanostructures¹

ZHENYU ZHANG, Oak Ridge National Lab

Multiscale modeling is gaining an increasingly important role in guiding the fabrication of artificially structured nanomaterials with atomic-scale precision and desirable physical properties. In this talk, two recent examples will be presented to illustrate its predictive power in modern materials research. The modeling approaches range from electronic-scale calculations based on first principles to mesoscopic-scale continuum elasticity theory. Specific examples include: (a) fabrication of ordered magnetic atom wires on non-magnetic metal substrates; (b) optimal dopant control in dilute magnetic semiconductors via “Subsulfur Epitaxy.” Emphasis will be made on the substantially improved structure-property relationships achieved through such synergetic efforts between theory and experiment, including in the second example the striking observation of magnetic ordering temperatures well above 300 K.

¹Supported by USDOE, USNSF, & NSF of China, in collaboration with W.G. Zhu, Y.N. Mo, C.G. Zeng, J.D. Guo, K. Varga, E.G. Wang, H.H. Weitering, and E. Kaxiras.