Physics Ph.D. Defense

2:10 pm, Monday, May 12th, 2008

Room G26, Spaulding Hall

Surface structure and composition determination by a novel application of low-energy electron scattering and Monte Carlo simulations

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In this presentation I will report on a novel surface analysis technique that combines the strength of low-energy electron diffraction and microscopy, LEED and LEEM. This work is motivated by the quest in new nanotechnologies to be able to control the heterogeneity in ultrathin films, and the lack of surface sensitive techniques that can measure the crystalline geometry and composition with the necessary high lateral resolution. I will present a novel low-energy electron microscopy intensity-vs-voltage, or LEEM-*IV*, analysis technique and show that it is able, for the first time, to provide 3D structural maps of the surface region with nanometer resolution. In the dynamical *IV* analysis, a proper model of the multiple-scattering potential, representing the atomic muffin-tin and the inelastic optical scattering, was adapted to overcome the challenges in very low-energy electron scattering. In the presented studies of a model system, the well-known PdCu surface alloy grown on the (001) surface of copper I will quantify the temporal and spatial evolution of the Pd concentration on the Cu(001) terrace during the growth process and identify a step flow growth mechanism as the origin for the heterogeneity in the ultrathin alloy film. I will demonstrate in detail how 3D mapping of the Pd concentration profile in the surface region with a resolution of 8.5 nm is achieved and how Monte Carlo simulations can be used to predict the time evolution of the compositional heterogeneity. Furthermore, I will highlight a LEEM single domain diffraction analysis of the structure of the (0001) surface of 6H silicon carbide and the observed surface phase transitions. These results will further our understanding of the formation of graphene sheets on surfaces.