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C C M S C O L L O Q U I U M

An island dynamics model to describe strain induced ordering during heteroepitaxial growth

by

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Abstract: Epitaxial growth is a process where one crystalline material is deposited on top of a different crystalline material. It is a process that is relevant for the fabrication of many opto-electronic devices and nano structures. Different materials often have a mismatch of their natural lattice constants and strain arises in the system. For example, Silicon and Germanium, which are 2 important semiconductor materials, have a lattice mismatch of 4%. Such strain is often the driving force behind the formation and self-organization of nano features such as so-called quantum dots during epitaxial growth. It is therefore of paramount importance to understand and to be able to model epitaxial growth of strained system. In this talk we will discuss a model for epitaxial growth that employs an island dynamics model with the level-set technique in combination with a fully self-consistent elastic model, and that uses input for microscopic parameters that are obtained from essentially parameter free, quantum mechanical density-functional theory (DFT) calculations. First, we will present DFT calculations that examine the effect of strain on a number of microscopic growth parameters, such as adatom diffusion, dissociation of small islands, detachment of adatoms from islands, and diffusion of adatoms along island edges. We use growth of Ag on the Ag(100) surface as our model system. We then present results for several growth phenomena using our island dynamics model, e.g. in the submonolayer growth regime strain leads to more size uniformity of the growing structures. We discuss how one can exploit this effect of strain and can control the alignment and uniformity of the growing nanostructures. Specifically, we discuss how buried defects effect the mobility of adatoms, thus leading to ordering, and how stacked quantum dots are formed.

About the speaker: Christian Ratsch grew up in Berlin, Germany, where he received his undergraduate education at the Technical University. He then moved to the United States, where he completed his Ph.D. in physics at Georgia Tech in 1994. He went on to gain a short appointment at the Imperial College in London, and then a 2 year post-doc at the Fritz-Haber-Institut in Berlin. Ratsch came to Southern California in the summer of 1997. He worked first at HRL Laboratories in Malibu, and came to the UCLA Math Department in 2000. He has served as the Associate Director for the Institute for Pure and Applied Mathematics (IPAM) since the summer of 2006. Ratsch's research interests are mathematical and physical modeling and simulation of problems in materials sciences on all appropriate time and length scales. His expertise includes density-functional theory (DFT), stochastic, atomistic models (KMC), and continuum type models (level-sets).

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Freeburg Forum (Kravis Center, LC 62), Claremont McKenna College

Refreshments at 4:00 p.m. in Freeburg Forum Courtyard & wine and cheese after the talk in CMC Math Commons Room (Adams 208)

The dinner will be hosted by Prof. Robert Borrelli.
Please contact Prof. Borrelli if you are interested in attending the dinner.