Section 3  Surfaces and Interfaces

Chapter 1  Statistical Mechanics of Surface Systems and Quantum-Correlated Systems

Chapter 2  X-Ray Diffuse Scattering

Chapter 3  Semiconductor Surface Studies

Chapter 4  Ultralow Temperature Studies of Nanometer Size Semiconductor Devices

Chapter 5  The Quantum Hall Effect in Narrow MOSFETs

Chapter 6  Epitaxy and Step Structures on Semiconductor Surfaces
Chapter 1. Statistical Mechanics of Surface Systems and Quantum-Correlated Systems

Academic and Research Staff
Professor A. Nihat Berker, Dr. Joseph O. Indekeu

Graduate Students
William Hoston, Kenneth Hui, John F. Marko, Roland Netz

Undergraduate Students
Joseph E. Hilliard, Galen T. Pickett

Technical and Support Staff
Imadiel Ariel

1.1 Introduction

Sponsor
Joint Services Electronics Program
Contract DAAL03-89-C-0001

Correlated fluctuations play an important role in systems with electronic and structural degrees of freedom. This role is most ubiquitous at phase transitions, but is also considerable away from phase transitions, extending down to the lowest temperatures due to quantum mechanics. The renormalization-group method is a new calculational method that can systematically deal with correlated fluctuations at each successive scale length. Since we can include even the consequences of defects, for the first time we can obtain predictive microscopic theories for realistic systems.

1.2 Finite-Temperature Phase Diagram of Vicinal Si(100) Surfaces

Project Staff
Professor A. Nihat Berker

With the collaboration of Professor John D. Joannopoulos and Dr. Oscar L. Alerhand, we have combined electronic energy calculations and such statistical mechanics to obtain ab initio descriptions of finite-temperature semiconductor surfaces and interfaces. The entropy, free energy, and other properties have been evaluated for the silicon (100) surface. The single-step/double-step phase diagram in the variables of crystal cut angle and temperature, as well as other observable properties such as step profiles, are predicted in very good agreement with ongoing experiments. Contrary to previous suggestions that only double-layer steps should appear on the equilibrium surface, it is predicted that the single-layer stepped surface is at equilibrium for small misorientation angles. This structure is stabilized by strain relaxation and by the thermal roughening of the steps. For annealed surfaces, the critical angle at which the transition between the single- and double-layered stepped surface occurs is calculated to be $\theta_c \approx 2^\circ$.

1.3 Absence of First-Order Phase Transitions in Physical Surface Systems

Project Staff
Professor A. Nihat Berker, Kenneth Hui

Most recently, we made a theoretical prediction using the renormalization-group method that appears to have general and far-reaching consequences: we discovered that even an infinitesimal amount of randomness in interactions (e.g., distribution of defects) in
surface systems, converts first-order phase transitions, characterized by discontinuities, to second-order phase transitions, characterized by infinite response functions. In bulk systems, as (calculable) threshold randomness is needed for this conversion to occur. This general prediction appears to be supported by experiments on doped KMnF₃.

1.4 New Orderings in Systems with Competing Interactions

Project Staff
Professor A. Nihat Berker, William Hoston, Roland Netz

Our studies of realistic, complex systems with competing interactions have led to several new results. We have recently developed a new method that blends Monte Carlo simulation and mean-field theory. We are able to distinguish, for the first time, the effect of dimensionality on frustrated magnetic systems. We have obtained two ordered phases that nevertheless have considerable entropy. Also, we have recently obtained novel phases and multicritical points in systems with competing dipolar and quadrupolar interactions.

Publications


