Section 3 Surfaces and Interfaces

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 $\theta_c \approx 2°$.

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 reponse 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 $KMnF_3$.

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

Alerhand, O.L., A.N. Berker, J.D. Joannopoulos, D. Vanderbilt, R.J. Hamers, and J.E. Demuth. "Finite-Temperature Phase Diagram of Vicinal Si(100) Surfaces." Submitted to *Phys. Rev. Lett.* (1989).

Berker, A.N. "Harris Criterion for Direct and Orthogonal Quenched Randomness." Submitted to *Phys. Rev. B* (1990).

Hilliard, J.E. *Monte Carlo Simulation of a One-Dimensional Ising System with Competing Interactions Using Domain Walls.* S.B. thesis, Dept. of Physics, MIT, 1989.

Hui, K., and A.N. Berker. "Random Field Mechanism in Random-Bond Multicritical Systems." *Phys. Rev. Lett.* 62:2507 (1989).

Hui, K. "Domain Wall Study of the Stacked Frustrated Triangular Lattice." Submitted to *Phys Rev. Lett.* (1989).

Hui, K. *Quenched Disorder and Competing Interactions in Spin Systems.* Ph.D. diss. Dept. of Physics, MIT, 1989.

Marko, J.F. *On Structure and Scaling at First- and Second-Order Phase Transitions.* Ph.D. diss. Dept. of Physics, MIT, 1989.

Marko, J.F. "Exact Pair Correlations in a One-Dimensional Fluid of Hard Cores with Orientational and Translational Degrees of Freedom." *Phys. Rev. Lett.* 62:543 (1989).

Marko, J.F. "First-Order Phase Transitions in the Hard-Ellipsoid Fluid from Variationally Optimized Direct Pair Correlations." *Phys. Rev. A* 39:2050 (1989).

McKay, S.R., and A.N. Berker. "Magnetization of the d-Dimensional Random-Field Ising Model: An Intermediate Critical Dimension." In *New Trends in Magnetism.* Ed. S.M. Rezende. Teaneck, New Jersey: World Scientific, 1989.

Pickett, G.T. *Asymptotic Behavior of the Spectrum of Generalized Dimensions in Multifractal Tree Growth.* S.B. thesis. Dept. of Physics, MIT, 1989.