6. Phase Transitions in Chemisorbed Systems

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6.1 Multicritical Phase Diagrams of Chemisorbed Systems on Nickel

Joint Services Electronics Program (Contract DAAG29-80-C-0104)
Robert G. Caflisch, A. Nihat Berker, James S. Walker

Multicritical phase diagrams are evaluated for oxygen on Ni (100), starting with adsorption-lattice models with competing interactions, including trio interactions. We use global mean-field theory and renormalization-group theory, which we have developed into an effective tool via prefacing transformations onto coupled Potts-lattice-gas models. Different types of phase diagrams are found, each exhibiting disordered, 2 x 2, and $\sqrt{2} \times \sqrt{2}$ phases, separated by first-order transitions at low temperatures and second-order transitions at higher temperatures. These phase diagrams are qualitatively distinguished by tricritical points, triple points, critical end-points, and, possibly, a novel bicritical point. Our renormalization-group results carry indications of possible nonuniversality of critical behavior. Fitting phase diagrams from experiments currently in progress to our theoretical results will provide the best determination to date of microscopic interactions. The variety of phase diagrams we obtained also motivate experiments with sulfur, selenium, or tellurium on nickel.

6.2 Improved Renormalization-group Calculations of Critical Exponents in Surface Systems

Joint Services Electronics Program (Contract DAAG29-80-C-0104)
James S. Walker, David Andelman, A. Nihat Berker

The Migdal-Kadanoff (MK) transformation is probably the most flexible renormalization procedure, applicable to models which are particulate and, therefore, readily connected to physical systems. However, this transformation has been at best semiquantitative. We have removed this shortcoming by developing a synthesis of this transformation and of perturbative series expansions. The approximate step of the transformation, instead of being performed in an ad hoc manner, is done by conserving free energies order by order. When tested on the Ising model, the results are vastly

improved, as seen from the critical exponent values $\nu = 1, 1.34, 1.02$, from the exact, simple MK, or improved MK calculations. The approach is also being tested on Potts models, and will be of importance in predicting multicritical phenomena in surface systems.