

## 8. Phase Transitions in Chemisorbed Systems

### Academic and Research Staff

*Prof. A.N. Berker, Dr. J.O. Indekeu, Dr. M. Kaufman, Dr. M.P. Nightingale*

### Graduate Student

*S.R. McKay*

### Undergraduate Student

*S.I. Chase*

## 8.1 Selenium Chemisorbed on the Nickel (100) Surface

*Joint Services Electronics Program (Contract DAAG29-83-K-0003)*

*A. Nihat Berker, Robert G. Callisch<sup>8</sup>*

An experimental study, using high-energy electron diffraction, was recently done on selenium chemisorbed onto the nickel (100) surface. A phase diagram exhibiting  $c2 \times 2$  and  $p2 \times 2$  ordered phases was obtained. Based on this macroscopic observation, the authors of this work have premised the highly interesting Ashkin-Teller (non-universal) criticality to the corresponding phase boundaries.

We have constructed a microscopic theory for selenium on nickel (100) and found that the Ashkin-Teller symmetry is violated in several ways. Furthermore, these violations appear to grow under renormalization-group transformations. Thus, a massive reinterpretation of the phase diagram appears to be necessary. We are accordingly pursuing this prefacing/renormalization-group study. First, possible topologies of overlayer phase diagrams will be determined, using all reasonable combinations of Se-Se interactions. Secondly, actual Se-Se interactions will be estimated from new electronic calculations, in a collaboration with Prof. J.D. Joannopoulos. The corresponding phase diagram will be calculated in detail by renormalization-group. Additionally, our microscopic analysis has led us, in collaboration with Prof. A. Aharony (Tel Aviv University, to be at M.I.T. in 1986), to derive a Landau-Wilson free energy with terms heretofore ignored. A close analogy is thus discovered with the "dangerous irrelevant variables" of structural phase transitions.

---

<sup>8</sup>Schlumberger-Doll Research

## 8.2 Modified Hyperscaling Relation for Phase Transitions under Random Fields

*Joint Services Electronics Program (Contract DAAG29-83-K-0003)*

*A. Nihat Berker, Susan R. McKay*

Substrate imperfections locally differentiate between chemisorption sublattices, thereby creating a random-field situation for the epitaxial ordering. The random-field problem is of immense current and unresolved interest in many aspects of condensed matter physics and information sciences. We have conducted<sup>1</sup> a renormalization-group analysis for the internal energies near a second-order phase boundary under random fields, presuming flow to a strong-coupling fixed point. We have thus derived a modified hyperscaling relation,  $2-\alpha = (d-y_-)\nu$ , where  $\alpha$  and  $\nu$  are the critical exponents for specific heat and correlation length,  $d$  is dimensionality, and  $y_-$  is the strong coupling runaway eigenvalue exponent of our theory. We find the bound  $y_- \leq d/2$  for order parameters of arbitrary number of components. This result is of application to currently reported competing experimental results on critical exponents.

## 8.3 Random-Field Critical Behavior

*Joint Services Electronics Program (Contract DAAG29-83-K-0003)*

*Miron Kaufman*

Heat capacity data from the random-field system  $\text{Fe}_{1-x}\text{Zn}_x\text{F}_2$  is considered.<sup>2</sup> The Ginzburg criterion for the onset of critical behavior is thus extended to random-field systems. It is argued that the failure of the supersymmetry formalism prediction of dimensional reduction by two is due to the divergence of thermal fluctuations in less than four dimensions. A droplet model for random fields is developed, which predicts a first-order transition for any infinitesimal random-field in the neighborhood of the zero-field critical point.

## 8.4 Renormalization-Group Analysis of Heat-Capacity Critical Amplitudes

*Joint Services Electronics Program (Contract DAAG29-83-K-0003)*

*Scott I. Chase, Miron Kaufman*

Critical amplitudes  $A_{\pm}$  associated with the temperature ( $t$ ) variation of the heat capacity  $C \sim A_{\pm} |t|^{-\alpha}$  are analyzed by means of renormalization-group techniques in both position and momentum spaces.<sup>3</sup> We have found a mechanism by which the amplitudes  $A_{\pm}$  diverge as the critical exponent  $\alpha$  approaches a nonpositive integer. In between two consecutive divergences at

least one amplitude vanishes at least once. The coefficient  $P$  in the expansion  $A_+/A_- = 1 - P\alpha + O(\alpha^2)$  is computed by means of  $\epsilon$ -expansion and Migdal-Kadanoff renormalization-group techniques. Systems for which  $0 > \alpha > -1$  exhibit either a cusped heat capacity if  $A_+/A_- > 0$  or a smooth heat-capacity maximum away from the critical temperature  $T_C$  and an infinite slope at  $T_C$  if  $A_+/A_- < 0$ . Implications of this result to the interpretations of experiments on random-bond systems such as  $Fe_{1-x}Zn_xF_2$  are presented.

## 8.5 N-Color Spin Systems in the Large N Limit

*Joint Services Electronics Program (Contract DAAG29-83-K-0003)*

*Miron Kaufman, Mahran Kardar<sup>9</sup>*

N-color order-parameter models are introduced and examined in the large N limit.<sup>4</sup> The free energy and critical properties at the phase transitions are studied. With relevant couplings between colors, the transition becomes either first order or Fisher renormalized. With irrelevant couplings, there is a changeover to first-order transitions through a nonclassical tricritical point. Connections are established between the N-color model, compressible systems, and systems with random impurities.

## 8.6 Wetting near Critical Points

*Joint Services Electronics Program (Contract DAAG29-83-K-0003)*

*M. Peter Nightingale, Joseph O. Indekeu*

We studied wetting phenomena in which the wetting layer is (nearly) critical and intrudes between two noncritical phases.<sup>5</sup> Finite-size scaling theory predicts an interaction, identical in range to that due to the van der Waals forces, between the interfaces bounding the wetting layer. This finite-size interaction leads to new wetting phenomena near critical endpoints, e.g., in ternary mixtures. The interaction amplitude and its possible universality can be observed directly in experiment.

Cahn's general argument for complete wetting in the vicinity of critical points is critically reviewed.<sup>6</sup> Critical-point wetting does occur in systems with short-range (exponentially decaying) forces. Whenever short-range forces favor wetting, while at the same time there is a tendency towards drying due to weak long-range (algebraically decaying) forces, neither critical-point wetting nor drying takes place. In this case, the thickness of the partial wetting layer diverges as the bulk correlation length upon approach of the critical point.

---

<sup>9</sup>Harvard University

### References

1. A.N. Berker and S.R. McKay, Phys. Rev. B 33, 4712 (1986).
2. M. Kaufman, in Superlattices and Microstructures, (Academic Press, London, 1985), Vol. 1, p. 511.
3. S.I. Chase and M. Kaufman, Phys. Rev. B 33, 239 (1986).
4. M. Kardar and M. Kaufman, Phys. Rev. B 31, 7282 (1985).
5. M.P. Nightingale and J.O. Indekeu, Phys. Rev. Lett. 54, 1824 (1985).
6. M.P. Nightingale and J.O. Indekeu, Phys. Rev. B 32, 3364 (1985).