Oxygen on Ni(111): A Transition of the Heisenberg Model with Cubic Anisotropy

Critical exponents of the transition to the $p(2\times 2)$ state observed in oxygen adsorbed on Ni(111) have recently been measured.[1] Under the assumption that the adsorption sites are threefold coordinated,[2] the ordered array is shown in Fig. 1. Because of a crystal field arising from subsurface layers of Ni atoms, the adsorption sites of the honeycomb array are not all equivalent but decompose into two interpenetrating inequivalent triangular arrays of fcc and of hcp sites. In this circumstance, the transition is in the universality class of the four-state Potts model.[3] However, the critical exponents measured in Ref. 1 ($\beta=0.14\pm 0.02$, $\gamma=1.9\pm 0.2$, $\nu=0.94\pm 0.10$) differ significantly from those of the four-state Potts model[4] ($\beta=\frac{1}{12}$, $\gamma=\frac{7}{6}$, $\nu=\frac{2}{3}$) but are equal within experimental error to those of the Ising model ($\beta=\frac{1}{8}$, $\gamma=\frac{7}{4}$, $\nu=1$). A plausible explanation is as follows.

If there were no crystal field, the transition would be in the universality class of the Heisenberg model with corner cubic anisotropy[3] [i.e., a ferromagnetic model of spins $\vec{S}=(S_x,S_y,S_z)$ with easy axes along the four cube diagonals]. The eight equivalent $p(2\times 2)$ ground states correspond to the eight states of this Heisenberg model, in which all spins point to any one of the corners of the cube. Grest and Widom[5] have recently shown that this model can exhibit a continuous transition which, over a finite region of the phase diagram, is governed by a marginally attractive decoupling fixed point of the three Ising models $S_\alpha=\pm 1$, $\alpha=x,y,z$. Thus, up to logarithmic corrections, the critical behavior of this transition is identical to that of the Ising model.

The addition of a crystal field in the experimental system is equivalent to the addition of a symmetry-breaking term $S_xS_yS_z$ into the Heisenberg model. This decomposes the eight equivalent ground states of the model into two inequivalent sets in which the spins point to the vertices of tetrahedra, one with the symmetry-breaking term positive, the other negative, and causes the transition to cross over from the class of the Heisenberg model with corner cubic anisotropy to that of the four-state Potts model.[3] The crossover exponent is large, $\phi=\frac{13}{8}$, indicating that the range of reduced temperatures t in which the four-state Potts exponents describe the critical behavior grows rapidly with increasing crystal field h, like $h^{8/13}$. Nevertheless, for any nonzero t the Heisenberg exponents describe the critical behavior for sufficiently weak fields. In the absence of detailed calculation, whether a given field is sufficiently weak is unknown. For the experiment in question, however, the answer can be inferred from the measured exponents.

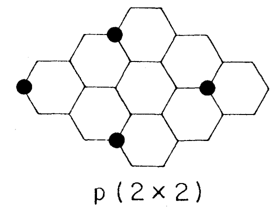

FIG. 1. $p(2\times 2)$ ordered array of O on Ni(111).

A plausible interpretation of the results of Ref. 1, then, is that the experiment has determined that the crystal field is small enough that the exponents measured are those of the Heisenberg model with corner cubic anisotropy and has confirmed that this model can exhibit continuous transitions with Ising exponents as indicated by Grest and Widom.[5]

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[1] L. D. Roelofs, A. R. Kortan, T. L. Einstein, and R. L. Park, Phys. Rev. Lett. 46, 1465 (1981).

[2] P. M. Marcus, J. E. Demuth, and D. W. Jepsen, Surf. Sci. 53, 501 (1975).

[3] E. Domany and M. Schick, Phys. Rev. B 20, 3828 (1979).

[4] The values quoted are those of the Baxter-Wu model, R. J. Baxter and F. Y. Wu, Phys. Rev. Lett. 31, 1294 (1973), which is in the same universality class as the four-state Potts model.

[5] G. S. Grest and M. Widom, private communication.