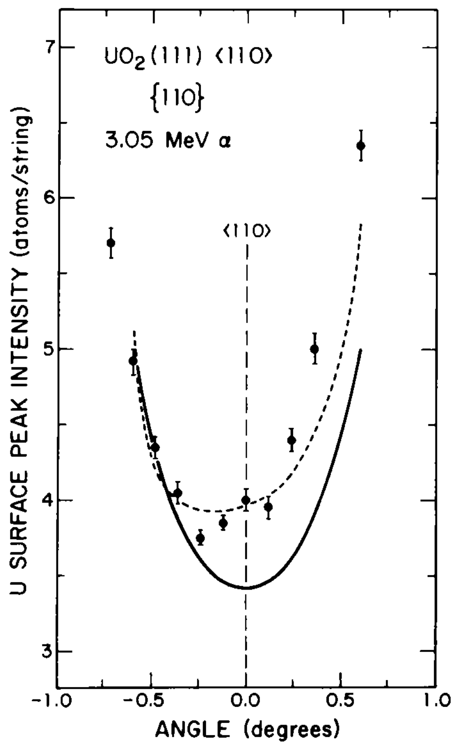

FIG. 1. $^4He^+/U$ rocking curve for the U surface peak near the ⟨110⟩ direction on the $UO_2(111)$ surface. Experimental data are individual points with error bars. Solid curve (—): ideal bulk termination, no surface vibrational enhancement or correlation. Dashed curve (---): 0.19 Å outward relaxation of the U surface layer, surface vibrational enhancement of 1.2 and no correlation.

like oxygen overlayer residing on an undistorted, underlying bulklike U lattice.[4] The present study addresses the possibility of U lateral distortions on this surface. Preliminary rocking curve data for the U surface peak, taken near the ⟨100⟩ direction for a $UO_2(100)$ vicinal surface [4.5° from (100)], show a symmetrical curve ~0.75 atoms/string larger than that expected for a simple bulk termination. Both surface vibrational enhancement and lateral distortion of U terrace atoms can be used to fit the data, although step effects may also play a role in the larger surface peak.

In summary, we have used RBS and Monte Carlo simulations to demonstrate an outward U surface layer relaxation for the $UO_2(111)$ surface.

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Summary Abstract: Relationship between many-parameter lattice gas systems and simpler models: Easy approximations for T_c

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While lateral interactions between chemisorbed atoms markedly affect many properties of the overlayer, they resist quantitative measurement because of their small size relative to binding energies and diffusion barriers. A powerful way to probe the interactions is to measure the 2-*d* phase diagram of the overlayer. The lateral interactions can then be treated as adjustable parameters in theoretical calculations (most often Monte Carlo) of the phase diagram.[1–5] In this procedure it is typically necessary to limit the number of parameters (and values for each). Thus, it would be useful to have a method, given T_c for one (typically small) set of interactions, to estimate T_c for a system of the same symmetry for a different (typically larger) set. We have found such a scheme[2,4] which is remarkably accurate for simple lattice gases for a wide choice of lateral interactions.

We describe the use of this method in terms of a $c(2\times2)$ overlayer on a square lattice, as shown in Fig. 1. A $c(2\times2)$ overlayer forms when there is a repulsive first neighbor interaction energy E_1. If this is the only interaction, the problem translates directly into the zero field Ising model, for which $E_1 \cong 1.76\ kT_c$,[6] shown as Onsager solution in Fig. 1. However, in real systems there are also longer range interactions, for instance, a second neighbor interaction E_2, as shown in Fig. 1. To determine the change in T_c caused by the addition of E_2, we consider the minimum energy required for an atom to move from an ordered site. As indicated by the ×'s in Fig. 1, the central atom can disorder most easily into a nearest neighbor site. If $E_2 = 0$, the energy cost for this move is $3E_1$, since there is no repulsion from the newly formed vacancy at the "central" site. (In contrast, in mean field the-

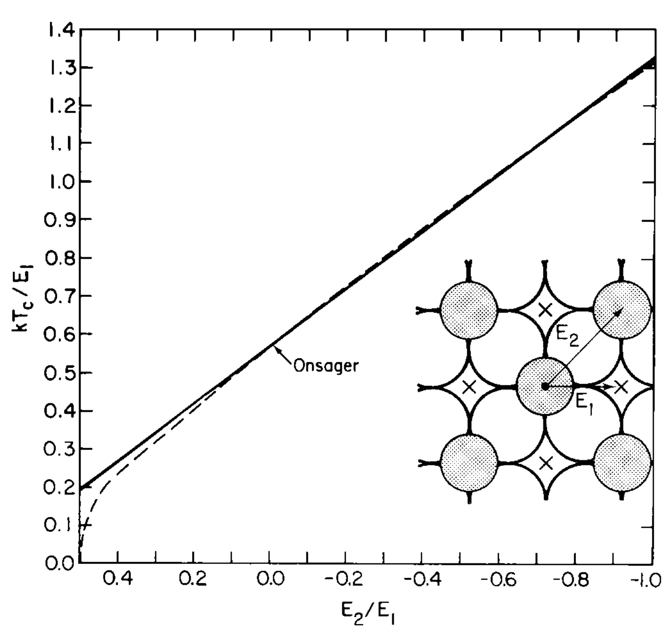

FIG. 1. Inset: $c(2\times 2)$ overlayer on a square lattice of adsorption sites. The lowest energy excitation for the central atom is into one of the four sites marked by $\times$'s. Graph: Transition temperature as a function of the second neighbor interaction energy for a $c(2\times 2)$ overlayer on a square lattice. Solid line: Eq. (1). Dashed line: Transfer matrix scaling calculation (essentially exact).

ory the adatom goes to a random vacancy with initial excitation energy $4E_1$.) If $E_2 \neq 0$, the energy cost is $3E_1 - 4E_2$. We then scale T_c using these excitation energies as follows:

$$\frac{3E_1 - 4E_2}{T_c(E_2)} = \frac{3E_1}{T_c(0)}$$

or

$$T_c(E_2) = T_c(0)\left(1 - \frac{4}{3}\frac{E_2}{E_1}\right). \tag{1}$$

This approximation is plotted in Fig. 1 along with essentially exact values obtained by transfer matrix scaling[7] calculations.

Equation (1) works extremely well in the range $-1.0 \leqslant E_2/E_1 \leqslant 0.1$. The mechanisms of its failure outside this range illustrate important restrictions on the use of the excitation scheme to predict T_c. First consider the case where $E_2/E_1 \geqslant 1/2$. Here the $c(2\times 2)$ structure with ground state energy $4E_2$ per adatom becomes unstable with respect to a (2×1) structure with ground state energy $2E_1$ per atom. Clearly, to use the excitation scheme the added interactions must not change the symmetry of the overlayer. In the range $0.1 < E_2/E_1 < 1/2$ the impending symmetry change at $E_2/E_1 = 1/2$ complicates the prediction of the minimum energy required to move an atom (i.e., multiatom moves evidently become important) causing the approximation to fail. The excitation scheme for E_2 strongly attractive ($-E_2 \gg E_1$) fails for a different reason. In this case the nearest neighbor repulsion becomes unimportant compared to the second neighbor attraction, and disordering into one of the sites marked by $\times$'s is not favored over disordering into a random site. In short, the excitation scheme can be used only if the minimum-energy disordering move is significantly lower in energy than any other possible move.

The excitation scheme can be used for lattice gas systems with a variety of symmetries and hence with different sets of interactions than discussed here, for instance, the $(\sqrt{3}\times\sqrt{3})$ $R\ 30°$ and (2×2) overlayers on a triangular lattice, the (2×2) on a honeycomb lattice, and the (2×1) on a bcc (110) lattice. In addition, it can be used to estimate the effects of trio (nonpairwise) interactions[8] on the phase diagram. A discussion of these applications, detailing their accuracy and their range of reliability, will be presented elsewhere.[9]

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