Multisite Interactions in Lattice-Gas Models of Adsorbates: Reconciling Adatom Relaxations at Steps

T.L. EINSTEIN, RAJESH SATHIYANARAYANAN, T.J. STASEVICH, U. of Maryland — In a lattice-gas (LG) framework for (111) cubic surfaces, pair interactions cannot distinguish A and B steps, but an orientation-dependent three adatom (trio) interaction can, as we verify with VASP for Cu(111). However, on Pt(111), small clusters considerably underestimate the difference. For a sequence of overlayer configurations, we explore the role of lateral relaxations and how they complicate LG analysis. On Cu(100) our prior VASP calculations of a particular trio interaction energy ($E_d$) gave a large positive value. This nearly cancels the attractive second-neighbor interaction energy ($E_2$), leading to a discrepancy between theory and experiment of step stiffness anisotropy. Relaxations at step edges greatly reduce this repulsion. Since position-dependent interactions are improper in LG models, we show how to deal with this phenomenon using a quarto interactions. We comment on extensions to (110) faces and analytic expressions for step stiffness.

1Supported by NSF MRSEC Grant DMR 05-20471, partially by DOE CMSN DEFG0205ER46227. Computing done at NCSA (NSF), UIUC.
2Now at Lab Receptor Biology, Nat’l Cancer Inst., NIH, Bethesda
3TJS et al., PRB a)70(‘04)245404, b)71(‘05)245414, c)73(‘06)115426.
4Feibelman, Surf. Sci. 463(‘00)L661; Michely et al., ibid. 256(‘91)217.

Theodore Einstein
University of Maryland, College Park

Date submitted: 20 Nov 2006