Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Vibrational spectroscopy and *ab initio* dynamics of the O-induced *added-row* reconstructed Cu(110) surface.[1] TALAT S. RAHMAN, M. ALCANTARA ORTIGOZA, University of Central Florida, R. HEID, K.P. BOHNEN, Forshungszentrum Karlsruhe, K. BRUEGGEMANN, H. IBACH, Forshungszentrum Juelich — It is known that O_2 molecules dissociatively adsorb on Cu(110) and, upon subsequent annealing, Cu and O atoms catenate along the [100] direction arranging themselves in a striped periodic super-grating, depending on O coverage and annealing temperature. It has been proposed that stress along the [110] direction in the regions that locally hold a (2x1)O added-row structure causes the formation of the stripes. Our electron energy loss spectroscopy (HREELS) and density functional perturbation theory calculations show however that the Rayleigh wave softens along the [110] direction, providing no indication that stress relief drives the formation of the stripes. Nonetheless, our calculations show also the stiffening of an in-plane mode which is peeled off above the bulk band and signifies strong O-induced intralayer force constant stiffening. Furthermore, HREELS at the Γ-point of the striped phase shows different degrees of softening of the O vertical mode, suggesting a stress relief gradient from the center of the stripes to the edges. Support to this interpretation is provided by our calculated phonon dispersion along the [110] direction of the O(3x1) added-row structure in which the O vertical mode appears softened with respect to that in the O(2x1) structure.

[1]Work supported in part by NSF under grant CHE-0548632.

Talat Rahman
University of Central Florida

Date submitted: 28 Dec 2007 Electronic form version 1.4