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Insights from surface stress calculations on the structure of c(2×2)-N overlayer on Cu(001)[1] SAMPYO HONG, TALAT RAHMAN, University of Central Florida — We present results of calculated changes in surface stress for N overlayers on Cu(001), in an effort to discriminate between several proposed structural models. Our calculations of the surface geometry and electronic structure are based on the density functional theory in the generalized gradient approximation and the pseudopotential method. We find that a c(2×2) N overlayer causes a large change in the surface stress ($\approx$ 5 N/m) on Cu(001) turning it from tensile to compressive. We also perform calculations for several stress relief models to find that the so-called "rumpling" and "clock reconstruction" models fail to relieve the N induced stress. On the other hand, formation of strips of clean Cu(001) areas, aligned along the $\langle 100 \rangle$ direction, and trench-like steps of Cu atoms, along the $\langle 110 \rangle$ direction on Cu(001), relieve the induced stress most effectively, in agreement with predictions from experiments. We consider the implications of these results on surface phonon dispersion curves for unreconstructed c(2x2)-N/Cu(001), which are in good agreement with experiment.

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