

# Temperature Dependence of the Ag(111) Surface Relaxation: An X-ray Reflectivity Study

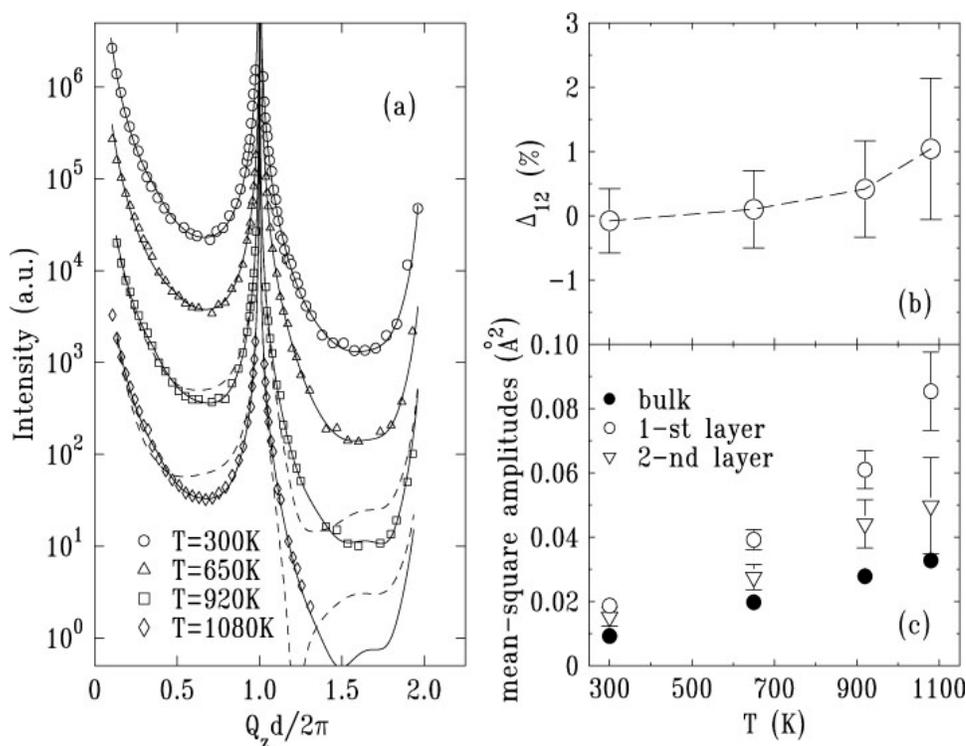
C.E. Botez, W.C. Elliott, and P.F. Miceli (U. of Missouri-Columbia) and P.W. Stephens (SUNY, Stony Brook)

Abstract No. bote8656

Beamline(s): X3B2

The anomalously large outward relaxation of Ag(111) observed by medium-energy ion-scattering (MEIS) [P. Satiris *et al.*, Phys. Rev. Lett. **72**, 3574 (1994)] has led to extensive theoretical investigations of this surface. Surprisingly, there is a persisting disagreement between the results from different theoretical methods: while molecular dynamics (MD) simulations indicate that the interlayer separations at the surface are almost bulk-like at all temperatures, quasiharmonic approximation (QHA) calculations predict a large high-temperature surface expansion. Motivated by this controversy, we measured the relaxation of Ag(111) surface within the temperature interval between 300 and 1100K (90% of the bulk melting point), using synchrotron x-ray diffraction, a technique that is well known for its ability to accurately determine the surface and bulk lattice-spacings simultaneously. Our specular reflectivity data show no evidence of a large surface expansion. At all temperatures we find that the first and second interlayer separations at the surface,  $d_{12}$  and  $d_{23}$ , differ from their bulk counterpart,  $d$ , by less than 1%, indicating that the surface is virtually unrelaxed relative to the underlying bulk crystal. This behavior is in good agreement with results from MD simulations, whose predictions for the surface vibrational amplitudes are also consistent with our experimental determinations.

Support is acknowledged from the NSF, under contract DMR-9623827 and MISCON under DOE grant DE-FG02-90ER45427. The SUNY X3 beam line is supported by the DOE, under contract DE-FG02-86ER45231 and the NSLS is supported by the DOE, Division of Material Sciences and Division of Chemical Sciences.



**Figure 1.** (a) Specular reflectivity of Ag(111) at four different temperatures. The dashed lines, which correspond to a large surface relaxation as predicted by the MEIS experiment, are not consistent with our data (open symbols) (b) The relaxation of the first interlayer spacing,  $\Delta_{12}=(d_{12} - d)/d$ , remains small ( $\leq 1\%$ ) at all temperatures. (c) The vibration amplitudes for the atoms in the top surface layers are enhanced with respect to their bulk counterparts, mainly at high temperatures.