Comment on "In-Plane Lattice Reconstruction of Cu(100)"

A low-energy electron diffraction (LEED) analysis of a clean Cu(100) surface, by Müller *et al.* [1], finds an in-plane lattice contraction of about 1%. Such an effect should be clearly visible in grazing incidence x-ray diffraction, but is not seen in our two independent sets of experimental data. In addition, systematic errors in LEED are generally accepted to be larger than the reported 1% effect.

The results of Müller *et al.* cannot differentiate between lateral contractions in different layers, giving only an average value. Thus, the actual surface could have a contracted top layer on an uncontracted substrate, or a gradual layer-by-layer decay of the contraction to the bulk lattice constant, or a thick uniformly contracted film to a depth beyond LEED penetration. Any of these models is inconsistent with our x-ray diffraction measurements for Cu(100), as shown in Fig. 1. Such contractions should cause a second displaced diffraction peak or at least an elongation or asymmetry of the main diffraction peak. Our experimental data in Fig. 1 show a radial scan across one of the crystal truncation rods (CTRs) of Cu(100) near the point of maximum surface sensitivity [2]. Under the chosen diffraction conditions, the penetration depth is more than 1000 Å; the CTR then includes contributions from both the surface and all bulk layers within this depth. The data show only one resolution-limited peak close to the position $q = 1$, as expected for an ideally terminated bulk lattice. Any of the above interpretations of the LEED result [1] would contribute a second component to the line shape displaced in q by 1%, as shown by the continuous curve in Fig. 1, calculated for a 1% contracted top layer. The resolution of our data is sufficient to exclude any 1% laterally contracted layer (within the penetration depth) as a component of the Cu(100) surface structure; even if a contracted top layer were considerably disordered, as suggested by the dashed curve, it should still contribute a pronounced asymmetry to the measured curve.

Regarding the reported LEED intensity analysis, the 0.02 Å effect is close to the quoted error bar (0.01 Å). As Müller *et al.* [1] state, this error bar describes only statistical uncertainties. They could not check all of the possible systematic errors. A round robin conducted on Cu(100) in 1987 [3] showed that systematic errors in LEED could then be as large as 0.03–0.07 Å. For comparison, systematic errors in bulk x-ray crystallography are often an order of magnitude larger than statistical errors [4]. Furthermore, discrepancies due to different *R* factors are typically on the scale of 0.01–0.03 Å for simple clean surfaces. Finally, several nonstructural parameters should have been optimized by Müller *et al.* [1], especially the atomic scattering potential.

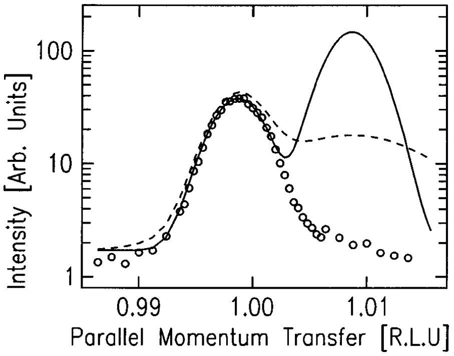

FIG. 1. X-ray diffraction measurements (circles) of a clean Cu(100) surface taken at X16A, NSLS. The scan is along the crystallographic direction $[q, q, 0.1]$, varying the momentum transfer component q parallel to the surface (expressed in reciprocal lattice units). X rays of energy 8.7 keV were used at an incidence and exit angle of 0.87°. The calculated curves are described in the text.

In conclusion, x-ray diffraction results do not confirm the reported lateral surface contraction, while the LEED analysis in question is most likely not accurate enough to establish such a contraction.

The authors acknowledge support under NSF Grants No. DMR93-15691 (I. K. R.) and No. DMR94-04421 (F. J.), BMBF Grant No. 055WMIBB8 (W. M.), and DOE Contracts DE-AC012-76CH00016 (I. K. R.) and DE-AC03-76SF00098 (M. A. V. H.).

I. K. Robinson,[1] W. Moritz,[2] F. Jona,[3] and M. A. Van Hove[4]
[1]Physics Department, University of Illinois
Urbana, Illinois 61801
[2]Institut für Kristallographie und Mineralogie
Universität München, Germany
[3]Department of Materials Science
State University of New York
Stony Brook, New York 11794-2275
[4]Materials Sciences Division
Lawrence Berkeley National Laboratory
University of California
Berkeley, California 94720

Received 12 December 1995
PACS numbers: 68.35.Bs, 61.14.Hg, 61.66.Bi, 68.10.Cr

[1] S. Müller *et al.*, Phys. Rev. Lett. **75**, 2859 (1995).
[2] I. K. Robinson, Phys. Rev. B **33**, 3830 (1986).
[3] F. Jona *et al.*, Surf. Sci. **192**, 398, 414 (1987).
[4] M. A. Van Hove *et al.*, Surf. Sci. Rep. **19**, 191 (1993).

0031-9007/96/76(19)/3659(1)$10.00