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In a recent Letter Schuster and Robinson [1] have published a determination of the surface relaxation of a homologous series of Cu(110) structures produced by adsorbing varying amounts of Cs. Increasing amounts of adsorbed Cs produces increasingly open missing row type reconstructions, and it is shown that the contraction of the interatomic distances at the surface increases strongly with the openness of the restructured surface. Schuster and Robinson speculate that polarization effects related to Smoluchowski smoothing play an essential role for the interlayer spacings and assert that simple methods like the effective medium theory (EMT) [2] or embedded atom method (EAM) [3] are incapable of giving a qualitatively reasonable description of the Cs-covered Cu(110) surface. Schuster and Robinson provide no experimental evidence for the polarization effects but try to argue based on the large relaxation calculated [4] for the clean (1×2) missing row (MR) reconstructed Au(110) surface with density functional theory (DFT) within the local density approximation (LDA).

In this Comment we present DFT/LDA calculations for the clean Cu(110) surface showing that Schuster and Robinson's speculation is not correct. The unreconstructed Cu(110) surface and the (1×2) MR reconstructed surface do in fact have rather similar spacings between the first two layers of the surface. This is also what is found in the EMT. The results of our calculations [5] are compiled in Table I. We find a contraction of the clean surface of 9% in excellent agreement with previous calculations and with experiment. The relaxation for the (1×2) missing row structure is only slightly larger, 10%. In the simple EMT the first layer is also found to contract, although by only 4% and the relaxation in the missing row structure is very similar.

In Table I we also include results for the other low index Cu surfaces and for the missing row (1×2) Au(110) surface. Experimentally, the more close packed surfaces are found to have smaller contractions than the Cu(110) surface, and this is reproduced both by the DFT calculations and the simpler EMT and EAM calculations. The missing row (1×2) Au(110) surface has a much larger contraction and this is again reproduced by DFT calculations [4] and the simple EMT. The large relaxations here are not a property of the missing row reconstruction, but primarily a material specific property.

The results presented here indicate that the experimentally observed relaxation pattern cannot be explained by just considering the properties of the clean surfaces, i.e., the adsorbed Cs may play a very active role in determining the surface relaxations. For the clean surfaces the DFT relaxation trends are well reproduced by the EMT even though the absolute error can be quite large.

TABLE I. The change Δd_{12} in the first interlayer spacing.

Δd_{12} (%)	Cu (110)	Cu (100)	Cu (111)	Cu-MR (110)	Au-MR (110)
LDA[a]	−9.1			−9.9	
LDA[b]	−9.27	−3.02	−1.27		−16
EMT[a]	−4	−2	−1	−5	−10
EAM[c]	−4.93	−1.44	−1.39		
LEED	−10[d]	−1.2[e]	−0.7[f]		−20[g]
Cs-Cu[h]	−4 ± 2			−14 ± 3	

[a]Present work.
[b]Reference [4].
[c]Reference [3].
[d]Reference [6].
[e]Reference [7].
[f]Reference [8].
[g]Reference [9].
[h]Deduced from Fig. 3 of Ref. [1].

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