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ATOMIC DISPLACEMENTS IN THE Au(110)-(1 × 2) SURFACE

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The Au(110)-(1 × 2) reconstructed surface was studied by high energy ion scattering. Measurements of the He^+ back scattering surface peak were made at 100 and 293 K as a function of energy (0.2 to 1.6 MeV) and crystal orientation. Comparison between measurements and calculations of the surface peak reveal that one monolayer of atoms is displaced in the surface plane by 0.12 ± 0.04 Å at 100 K and 0.18 ± 0.04 Å at 293 K. Assuming the missing row model, this corresponds to the second layer of atoms. Off-normal surface peak measurements give evidence for first layer displacements perpendicular to the surface.

There has been considerable progress in the understanding of the Au(110)-(1 × 2) surface in recent years. To explain the (1 × 2) LEED pattern which is due to a double periodicity along the [001] direction, three basic models, have been considered: "missing row", "pairing" and "buckling". The weight of recent results implies that either a missing row or a modified missing row model (i.e., with displacements) characterizes the basic structure [1–5]. In the missing row model, every other [$\bar{1}$10] close packed row is absent to expose close packed {111} facets. Since this simple missing row model could not explain the LEED I–V profiles, some modifications have been suggested such as first layer and/or second layer relaxation [2,4], second layer displacements and disorder [1,7,8]. Recently, the method of glancing angle X-ray diffraction established the existence of lateral displacements; in the context of a missing row model these displacements would be in the second layer [7]. Most recently, scanning tunneling microscopy [8] and electron microscopy [9] have mapped the Au(110)-(1 × 2) surface, clearly showing every other [$\bar{1}$10] row missing and some disorder and relaxation. It appears that the basic (1 × 2) missing row structure is now well established. In this paper we report measurements using high energy ion scattering which confirm the lateral displacement in this structure and give additional evidence for a vertical displacement of the first layer.

Ion scattering experiments were performed in a UHV system equipped with LEED and Auger apparatus to characterize the surface cleanliness and order. The UHV system is directly connected to the Van de Graaf accelerator for ion

scattering/channeling analysis. The principle of ion scattering for surface structure analysis is explained elsewhere [10]. The same Au crystal which was used for glancing angle diffraction [7] was inserted into the UHV system. After a few cycles of sputtering and annealing at 350°C, that is below the phase transition temperature from (1 × 2) to (1 × 1) phase, a sharp (1 × 2) LEED pattern was obtained without any trace of impurities by Auger analysis.

The energy dependence of the surface peak of the Au(110) along the normal [110] direction is shown in fig. 1. Data sets were obtained at room temperature (circles) and 100 K (squares). (Note that at low temperature and low energy the surface peak approaches 1.0 atom/row. This represents a useful check on the calibration of the system and also demonstrates that the effect of ion beam damage is almost negligible over the scanned energy range.) Also shown in fig. 1 are measurements from another recent ion scattering study of this surface which emphasized analysis of the surface vibrations [11].

The surface peak yields were calculated by Monte-Carlo simulation [12]. Fig. 1 shows the calculated yields at 100 and 293 K for: (a) bulk-like termination and bulk thermal vibration (μ_b); (b) bulk-like termination with a

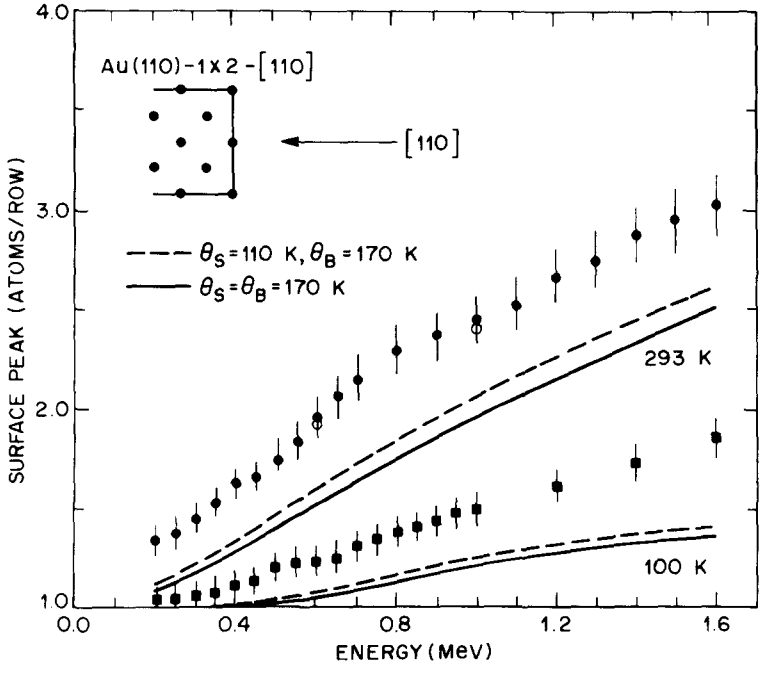


Fig. 1. Energy dependence of the [110] surface peak at 293 and 100 K. The full curves correspond to the results of computer simulations assuming a bulk structure and bulk vibration amplitudes (θ_b = 170 K). The dashed curve corresponds to a bulk structure and an enhanced amplitude (θ_s = 110 K) for the first layer. Also shown is a measurement (open circle) at 293 K from ref. [10].

typical enhanced surface vibration (μ_s) corresponding to an in-plane surface Debye temperature (θ_s) of 110 K for the first layer. In both cases, the equal time, nearest neighbor correlations from a Debye model are included, corresponding to the bulk Debye temperature (θ_b) of 170 K. The choice of $\theta_s = 110$ K was based on the results of the extracted surface Debye temperature from the recent X-ray measurements [7]. The substantial disagreement between calculation and observation can be due either to additional surface vibration or else to atomic displacements. In order to find the effect of the surface enhanced vibration we have calculated the surface peak yields for various surface Debye temperatures from 50 to 170 K. When θ_s is about 60 K, the calculated curves approach the measured data set. For this unusually low surface Debye temperature, the rms vibration amplitude $\mu_s \cong 2.9\mu_b$. The enhancement is high compared to the usual in-plane metal surface component $\mu_s \gtrsim \mu_{bulk}$ and inconsistent with the X-ray data. Thus we seek alternative explanations for the discrepancy between experiment and calculation (fig. 1) via surface atomic displacements.

The analysis of the displacement of the Au atoms depends on the difference between the measured surface peaks and the "known" calculated values. The uncertainty in the calculated values is primarily due to a lack of knowledge of surface vibration amplitudes. We have used the reported surface Debye temperature $\theta_s = 110$ K for the rest of the analyses. The displacement analysis is over the whole energy range, which obviously provides a higher confidence as compared to measurements on a single energy. Further we ascribe a higher confidence to the low temperature data where the affect of enhanced amplitudes is smaller (fig. 1).

For the [110] normal direction one atom/row corresponds to two monolayers. At high energies, where the shadow cone is less than the displacement, the difference between the experimental data and the bulk-like calculated curve is a measure of the number of displaced monolayers. In this case the difference is approximately 1/2 atom/row or one monolayer. In this geometry ion scattering cannot distinguish between displacements in the first layer or second layer. Fig. 2 compares the data with models corresponding to one monolayer (either the first or the second) displaced 0.12 and 0.18 Å and includes enhanced surface vibrations ($\theta_s = 110$ K). The quality of the fit was determined by minimizing the following quantity:

$$r^2 = \frac{\sum_{i=1}^{N} (Y_{th} - Y_{ex})^2}{N},$$

where N is the number of measured data points, and Y_{th} and Y_{ex} are the simulated yield and the measured yield, respectively. The low temperature data are well fit by a structure which assumes one monolayer of atoms displaced by

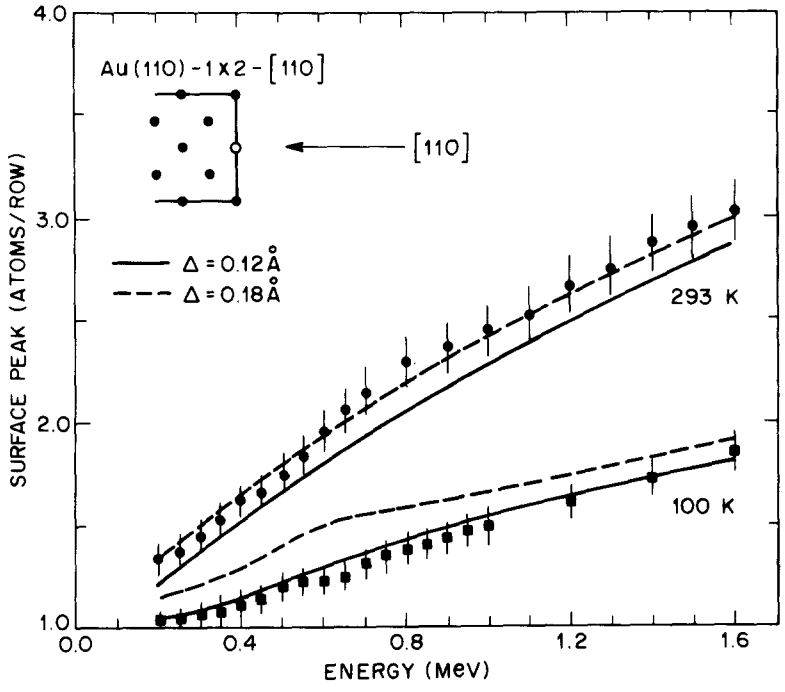


Fig. 2. Energy dependence of the [110] surface peak at 293 and 100 K. The curves correspond to the results of computer simulations assuming a full monolayer of atoms displaced 0.12 or 0.18 Å and includes enhanced surface vibrations ($\theta_s = 110$ K) in the first two layers.

0.12 ± 0.04 Å; the room temperature data by a displacement of 0.18 ± 0.04 Å. The apparent difference in the displacement at 100 and 293 K may be significant; however, the experimental error precludes a positive statement to this effect.

To illustrate the displacement in more detail, we plot the measured "extra monolayers" (i.e., the difference between the measured and surface peaks calculated for a missing row structure *without* displacements as a function of energy for the data taken at 100 K (fig. 3)). The data points fit the curve corresponding to a displacement of 0.12 Å. Other lines indicate the expected dependence for structures with one layer displaced by 0.10 and 0.15 Å, respectively. Note that if there is no displaced layer, the difference data will be scattered around zero if the surface Debye temperature is correctly chosen.

Figs. 4a and 4b show the energy dependence of the surface peak along the non-normal $[\bar{1}0\bar{1}]$ direction. The surface peak measurement along the non-normal direction is sensitive to displacements perpendicular to the surface. The square data points are for the surface at 100 K, and the circles are at room temperature. Calculated curves are shown for 100 and 293 K ($\theta_s = 110$ K) for a

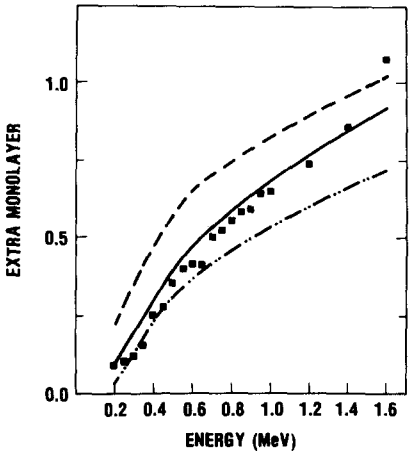
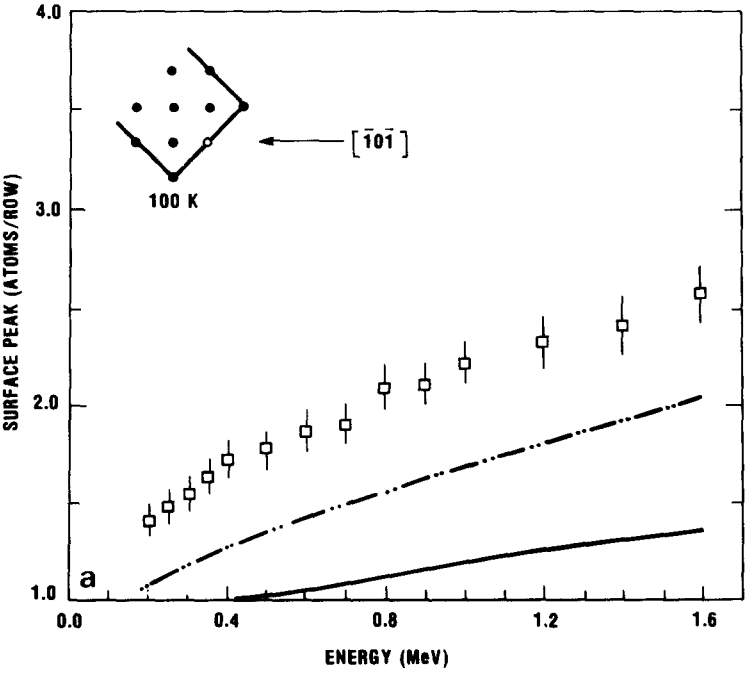


Fig. 3. Energy dependence of "extra monolayers", i.e. the difference between the experimental result and the "bulk-like" structure calculation. The curves correspond to displacement of 0.10 Å (– · · –), 0.12 Å (———) and 0.15 Å (— — —).



bulk-like surface and a surface with one monolayer displaced laterally. Clearly these values do not fit the data. All the data points lie about one half monolayer (in the $[\bar{1}0\bar{1}]$ direction 1 atom/row = 1 monolayer) higher than the calculated curves (which include lateral displacement). The difference of a half of a monolayer is due to perpendicular relaxation since it was not detected when the ion beam was directed along the normal direction. In the context of a missing row model the 1/2 monolayer relaxation probably corresponds to the first layer, which is the only half-filled one.

These results give definite evidence for a structure with one monolayer of atoms displaced laterally. In a model independent way this could be a complete first layer as in a first layer "pairing" structure and/or a specific combination of first layer and second layer displacements. In this paper we have shown that enhanced surface vibrations comprise a relatively small effect based upon the estimated vibration by X-ray measurement; the main factor is

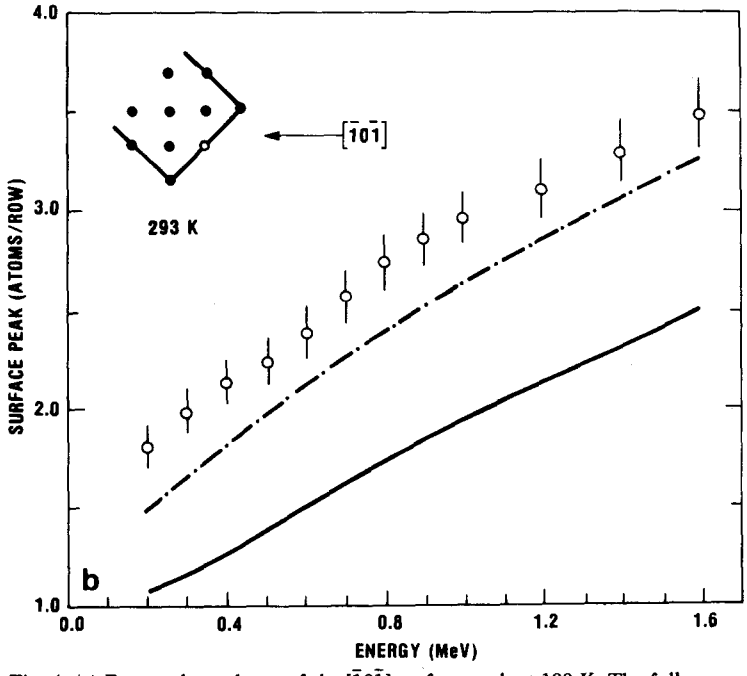


Fig. 4. (a) Energy dependence of the $[\bar{1}0\bar{1}]$ surface peak at 100 K. The full curves are for computer simulations assuming a missing row model with $\theta_s = 110$ K for the first and second layers. With those parameters the curves correspond to: (———) no lateral displacements and (— — —) lateral displacements of 0.12 Å in one full monolayer. (b) Energy dependence of the $[\bar{1}0\bar{1}]$ surface peak at 293 K. The full curves are for computer simulations assuming a missing row model with $\theta_s = 110$ K for the first and second layers. With those parameters the curves correspond to: (———) no lateral displacements and (— — —) lateral displacements of 0.18 Å in one full monolayer.

the rearrangement of surface atoms. The results are completely consistent with a missing row model as determined via electron and tunneling microscopy with second layer displacements observed by glancing X-ray diffraction. It is worth noting the good agreement between the measured surface peaks of Jackson et al. [11] and our results in the region of overlap (fig. 1). Since these authors noted a large difference between the Pt(110)-(2 × 1) and Au(110) surface, it would be interesting to apply other surface probes such as glancing X-ray diffraction to the Pt(110) surfaces.

In conclusion we have measured the parallel and observed the perpendicular displacements in the reconstructed Au(110)-(1 × 2) surface. Assuming a missing row model we find the second layer is displaced laterally by 0.12 ± 0.04 Å at 100 K and 0.18 ± 0.04 Å at 298 K, close to the value of 0.122 ± 0.017 Å (at 298 K) reported by X-ray scattering. In, addition the half-filled first layer is displaced perpendicular to the surface by more than ~ 0.25 Å. These results are entirely consistent with the modified missing row model and serve to quantify the atomic displacements.

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