14.2–1 STRUCTURAL STUDY OF THE TA(100) SURFACE AT EARLY STAGES OF OXIDATION. A.Titov and H.Jagodzinski, Institut für Kristallographie und Mineralogie, Universität München, Theresienstr.41, 8 München 2, FRG.

Oxidation of the Ta(100) surface was studied by LEED and Auger Spectroscopy. On evaporation of the oxide layers three ordered structures were observed, (3x3), (1x2) with satellites about all reflection and (1x3). A relation between O coverage and observed LEED structures was established by AES during O_2 adsorption. The (1x3)-O structure was analysed by comparing 11 experimental and theoretical I-E spectra. Since no satellites in LEED patterns of this structure were observed, an unit cell of a 2mm symmetry with 3 Ta atoms in the uppermost Ta layer was suggested. LEED intensities of models with and without Ta substrate reconstruction combined with an O layer in the possible binding sites were calculated. As a result a transformation of the uppermost Ta layer to buckled V-form Ta chains with following characteristics was concluded: the magnitude of buckling 0.10 Å and the lateral contraction of the Ta-Ta atomic distance 0.3 Å (a bulk value of the Ta unit cell - 3.30 Å). Thereby are the interlayer spacings between 1st and 2nd Ta layers 1.40± 0.05 Å and between 2nd and 3rd Ta layers 1.60± 0.05 Å. A model of quasi-tetrahedral binding sites for O atoms between 1st and 2nd Ta layers with the atomic distances of Ta(1)-O = 1.95± 0.05 Å and Ta(2)-O = 2.05± 0.10 Å has resulted in a minimal r-factor. Starting with the known binding site for an O atom in the (1x3)-O structure the models consistent with all AES and LEED data are proposed for the other two structures. According to these models a lowering of a symmetry of the (1x2)-O structure compared with the (1x3)-O structure inevitably leads to satellite patterns.

14.2–2 LEED-INVESTIGATION OF THE RECONSTRUCTED SI - (001) - SURFACE F. Kretschmar, H. Jagodzinski, D. Wolf
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The Si(001)-surface has long been known as reconstructed either in (2x1) or c(4x2). Recent work by Yang et.al. (Phys.Rev.B28, S.2049-1983) revealed a five layer distorted, horizontally and vertically asymmetric (2x1)-dimer model out of fulldynamically calculated LEED-I/E-spectra at best fit to experiment with r-factors below 0.2 - inspite of poor optical resemblance and Ni-stabilization.

Both structures, (2x1) and c(4x2), could be prepared using the same crystal, by slow cooling from 1600 K to 300 K (typically 1 K/s) and rapid cooling from 1600 K below 250 K (typically within 10 s), respectively. The c(4x2)-structure could not be kept stable at temperatures around 200 K, but changed to the (2x1)-structure as a consequence of decreasing c(4x2)-domain size. The structural phase transition as well as the order-disorder transition have been investigated both by LEED-I-V-measurements and LEED-beam profile analysis. The (2x1)-structure showed strong dependence on primary electron current even for values below 10^{-7} A, leaving LEED-spots sharp but reducing their intensity.
On the base of these experimental results a new model-conception of the Si(001)-surface has been developed, using "doubly" asymmetric dimer -blocks, corresponding both to the change from c(4x2) to (2x1) and instability of superstructures against external influences.

14.2–3 RECONSTRUCTION OF THE IRIDIUM (100) SURFACE DETERMINED BY LEED. By W.Moritz, F.Müller, D.Wolf and H.Jagodzinski, Institut für Kristallographie und Mineralogie der Universität München, Theresienstr.41, 8 München 2, FRG.

The (1x5) superstructure of the Ir(100) surface has been determined by LEED intensity analysis. The stable atomic arrangement of this surface consists of a distorted close packed layer in two bridge registry on top of a nearly undistorted second layer. The top layer is slightly compressed and exhibits a considerable buckling of about 0.5 Å, where the atoms in bridge positions are 0.3 Å below the topmost atoms. The lateral interatomic distances are in one direction about 3 % smaller than in the bulk, also the bond lengths to the atoms of the second layer are about 3 % reduced. The metastable unreconstructed (100) surface exhibits a slightly smaller reduction of bond lengths.

25 experimental I-V curves at normal incidence in the energy range from 30 to 220 eV were compared with theoretical spectra. All structural parameters within the reconstructed surface layer have been varied independently. The minimum average R-factors are 0.19 for the Zanazzi and Jona R-factor, and 0.39 for Pendry's R-factor.

The calculation of layer scattering matrices were performed using the matrix inversion method, and using symmetry adapted functions for the partial wave representation of the wave field within the layer. Only symmetrically independent atomic positions are needed in this case. The atomic potential was calculated relativistically and the crystal potential was obtained by superposition of the atomic potentials. In the multiple scattering calculations spin averaged phase shifts were used.

14.2–4 RECONSTRUCTION OF THE (100) SURFACES OF PT AND AU. By W.Moritz, Institut für Kristallographie und Mineralogie der Universität München, Theresienstraße 41, 8ooo München 2, FRG

The LEED pictures of the reconstructed surfaces of Pt and Au are qualitatively interpreted by two-dimensional anharmonic lattice distortions in the surface layer. The basic structure of the surface layer itself is assumed to be the same as in the (1x5)structure of Ir(100), which consists of a buckled quasi-hexagonal layer. The metastable (25x5) structures of Pt and Au(100) exhibit as a main feature a rectangular displacive modulation produced by regularly spaced partial dislocations and a compression of the layer perpendicular to the dislocation boundaries. In the thermodynamic stable surface of Pt the dislocation boundaries are slightly rotated, leading to a saw-tooth like displacive modulation.
The stable phase on Au(100) exhibits a centered longitudinal displacive modulation parallel to the dislocation boundaries. Very probably the combination of two perpendicular modulations leads here to a network of intersecting dislocation boundaries.
In these structure models the characteristic features of the diffraction pictures are produced by the surface layer itself, not by multiple diffraction. Multiple scattering effects in modulated surface structures can be analytically described by an amplitude modulation in addition to a displacive modulation. It is shown by model calculations that by multiple scattering more satellites occur than in the kinematic case, but the intensity distribution remains in the average qualitatively the same.
Consequently the satellites observed in the diffraction pictures of Pt and Au(100) should be caused rather by lattice modulations than by double or multiple diffraction, between the surface layer and the bulk.