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HYDROGEN-INDUCED RECONSTRUCTION OF STEPPED W(001) SURFACES STUDIED WITH LEED AND EELS

J. F. Wendelken and G.-C. Wang

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HYDROGEN-INDUCED RECONSTRUCTION OF STEPPED W(001) SURFACES STUDIED WITH LEED AND EELS*

J. F. Wendelken and G.-C. Wang**
Solid State Division, Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

Low energy electron diffraction patterns show that the W(001) surface reconstructs at room temperature when exposed to hydrogen with a $(\sqrt{2}x\sqrt{2})R45°$ structure having a c2mm symmetry.[1-3] Vibrational EELS data indicate that the tungsten atoms move together to form dimers[4] which must be aligned in <10> directions to satisfy the symmetry requirement.[2] The two possible dimer orientations define two orthogonal, degenerate domains. It has been shown that steps on a surface may limit the growth of the reconstruction domains and may also influence the relative abundance of the domain orientations.[1-3,5] We report here an extension of previous work on step effects involving the relationship of step orientation to domain growth and selection.

Results obtained for three W(001) surfaces are compared for this study. A planar surface was cut and polished to within 0.1° of the (001) while two stepped surfaces were prepared with alignments 3.25 ± 0.25° off the (001) with step edges perpendicular to the $[1\bar{1}0]$ in one case and to the [100] in the other case.[5] These steps, herein referred to as $[1\bar{1}0]$ and [100] steps, respectively, have an average separation of ~30 Å. All measurements on these three surfaces were performed in a single UHV system in which an EEL spectrometer was used for both LEED beam shape measurements, for which procedural details are presented elsewhere,[5] and vibrational measurements.

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**Present address: Physics Department, Rensselaer Polytechnic Institute, Troy, NY 12181.

Hydrogen adsorption on W(001) proceeds with two distinct reconstruction phases at room temperature.[2,3] In the LEED patterns from the commensurate phase on the planar crystal, broadening of the {1/2,1/2} LEED beams indicates an average domain size of ~123 ± 20 Å. Following the commensurate phase with increasing hydrogen exposure is an incommensurate phase characterized by a coverage dependent four-fold splitting of the half-order beams which results from a decreasing periodicity or domain wall separation. Measurements made on the planar crystal indicate a minimum periodicity of ~12 Å before the surface develops a (1x1)-H structure.

Step effects on domain shapes in the commensurate phase for the two stepped surfaces are illustrated schematically in Figure 1. In both cases, elongation of the half-order beams and their lack of splitting at any energy indicate that the reconstruction domains do not cross the step, but nearly fill the terraces, as previously reported for the surface with [1$\bar{1}$0] steps.[5] Parallel to the steps, the beams are also broadened indicating domain size limitations of just over 50 Å in both cases. This is surprising in view of our previous studies with the same two surfaces of the low temperature, clean surface reconstruction[7] in which the domain sizes parallel to the steps were found to be ~120 Å and 55 Å on the [1$\bar{1}$0] and [100] stepped surfaces, respectively. This difference was attributed to the high degree of domain selection on the [1$\bar{1}$0] stepped surface. With the hydrogen-induced reconstruction, selection of a single domain orientation is revealed in the incommensurate phase for the [100] stepped surface as reported by others[2,3] and indicated by the occurrence of two-fold

rather than four-fold splitting in the incommensurate phase. The reason for the domain size limitation parallel to the [100] steps is not clear, but may be associated with the fact that the hydrogen adsorption occurs initially on small clean surface p2mg domains which are degenerate on this surface.

Although it is clear that a single domain orientation is preferred with [100] steps, the orientation of that domain is less clear. King and Thomas[3] first addressed this issue and concluded on the basis of a periodic lattice distortion model that the dimers were preferentially oriented perpendicular to the step edges. But, Barker and Estrup[2] concluded on the basis of relative half-order beam intensities that the dimers must be aligned parallel to the steps and perpendicular to antiphase domain boundaries, or solitons, in the incommensurate phase. We have utilized EELS as indicated in Fig. 2 to examine this problem. As shown before, there are three hydrogen vibrations on W(001) which may be observed, and impact scattering rather than dipole scattering is the dominant scattering mechanism for the modes which are parallel to the surface.[4] It has been shown that, if a mode is observed by impact scattering and the scattering plane is a mirror symmetry plane, then that mode will not be observed, if its motion is perpendicular to the scattering plane.[6] In Fig. 2 we see that if we make observations parallel and perpendicular to the steps with the commensurate phase structure, ν_2 (wagging mode) and ν_3 (asymetric stretching mode), respectively, are emphasized in the spectra, implying a dimer orientation perpendicular to the steps. Measurements in progress on a surface with

[100] steps, but a 50 Å terrace width, indicate the same behavior. We note also that the ν_3 mode is much weaker on the stepped surfaces than on the planar surface. This may be a consequence of the dimer orientation, but further study will be required to verify this.

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FIGURE CAPTIONS

Fig. 1. Hydrogen induced reconstruction domain geometries on stepped W(001) surfaces.

Fig. 2. Azimuthal dependent EELS data for the commensurate phase of hydrogen-induced reconstruction on W(001) with [100] steps.

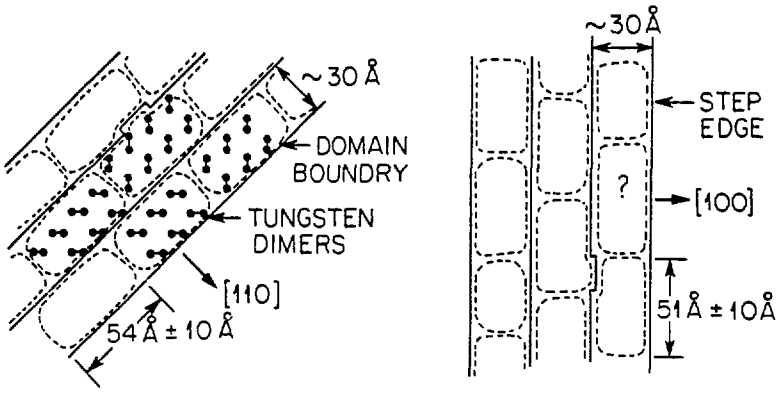
~30 Å
DOMAIN
BOUNDRY
TUNGSTEN
DIMERS
[110]
54 Å ± 10 Å
~30Å
STEP
EDGE
?
[100]
51 Å ± 10Å

Fig. 1

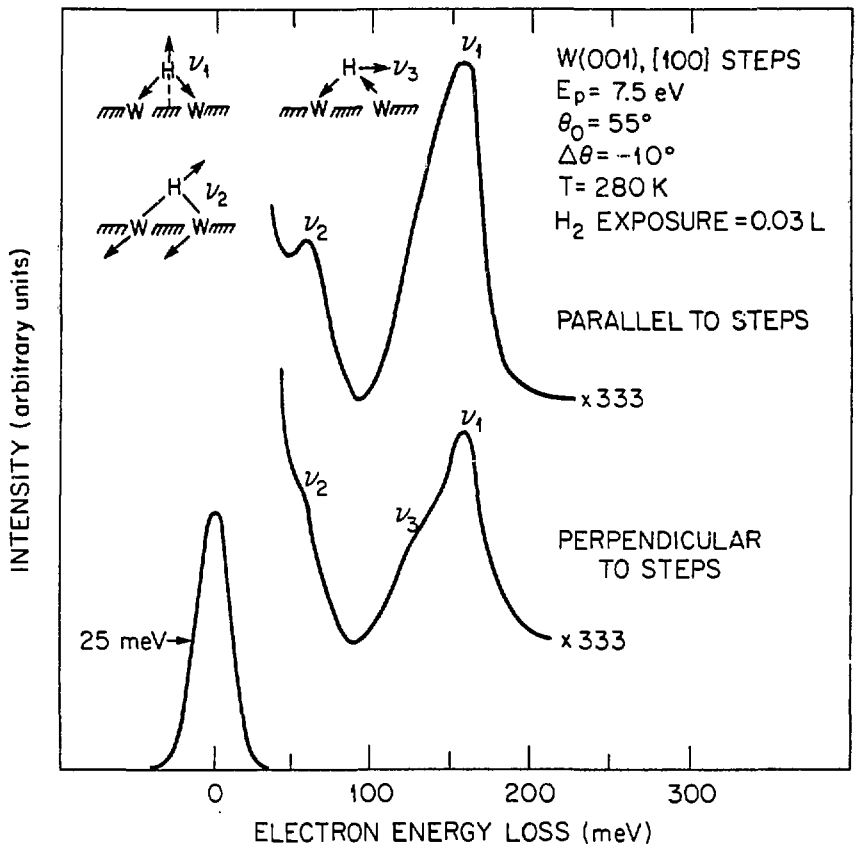
W(001), [100] STEPS
E_p = 7.5 eV
θ_0 = 55°
$\Delta\theta$ = -10°
T = 280 K
H_2 EXPOSURE = 0.03 L
PARALLEL TO STEPS
x 333
PERPENDICULAR TO STEPS
x 333
25 meV
ν_1
ν_2
ν_3
INTENSITY (arbitrary units)
0
100
200
300
ELECTRON ENERGY LOSS (meV)

Fig. 2