

converging wave guide, it has been concluded that such a guide reduces the major radius of the ring because of the magnetic flux compression between the wall and the ring.

To study the behavior of a confined ring, we have injected a 200-kA, a 30-nsec duration hollow beam through a cusp into a static field that is described by $B \sim (z/z_0)^{1.6}$. Upon passing the static compression magnetic field, the ring enters the magnetic mirror, where it is trapped. The trapping is achieved by raising the near-mirror peak using a gate field. The risetime of the gate field is much shorter than the one-way transit time of a typical proton between the peaks. It has been found that the ring is r - z stable for the entire time interval tested (about 550 nsec) after trapping in the mirror. Although the ring has an almost circular cross section at the midplane, near the mirror peaks its cross section is slightly elongated in the radial direction and it has an aspect ratio that is slightly smaller than unity. There are no radial or axial proton losses during the entire confining period tested.

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Space-Group Determination of the Low-Temperature $W\{001\}(\sqrt{2} \times \sqrt{2}) R45^\circ$ Surface Structure by Low-Energy-Electron Diffraction

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Low-energy-electron diffraction I - V spectra obtained from the clean, cooled $W\{001\}(\sqrt{2} \times \sqrt{2})R45^\circ$ surface structure at < 190 K display $2mm$ point-group symmetry, revealing a preferential orienting of equivalent domains. A further novel effect, that the half-order beam spectra ($\pm h/2, \pm h/2$) are identical in relative intensity to the ($\pm h/2, \mp h/2$) spectra but different in absolute intensity by a constant factor, uniquely establishes the space-group symmetry of the domains as $p2mg$. A structure for a single-layer surface rearrangement is proposed.

Recent investigations^{1,2} of the $(\sqrt{2} \times \sqrt{2}) R45^\circ$ surface structure of $W\{001\}$ produced by cooling below ~ 370 K, first reported by Yonehara and Schmidt,³ have established the structure as a clean surface phenomenon.

In this Letter we report on the first determina-

tion of the two-dimensional space-group symmetry of this surface structure, and an apparently unique structure for a top-layer rearrangement model. Low-energy-electron diffraction (LEED) I - V spectra from 24 half-order beams and 12 integral-order beams at normal incidence

clearly display a $2mm$ point-group symmetry. Since the diffraction pattern, including intensities, must show the same rotational symmetry as the substrate when the surface structure contains equal numbers of all its possible equivalent domains, the observed $2mm$ symmetry implies a preference for one rotational orientation over another of domains each having $2mm$ symmetry. A further novel effect, that the $(\pm h/2, \pm h/2)$ spectra and the $(\pm h/2, \mp h/2)$ spectra are identical in relative intensity but different in absolute intensity by a constant factor, can be explained by systematic absences of just the $(\pm h/2, \pm h/2)$ beams from each domain, so that a predominance of one domain orientation causes the $(\pm h/2, \pm h/2)$ beams to be uniformly weaker than the $(\pm h/2, \mp h/2)$ beams. The only two-dimensional space group satisfying these requirements is $p2mg$.

Details of the experimental setup have been briefly discussed before⁴ and will be more completely documented in a later publication.⁵ Pertinent to the following, however, is that the diffracted intensities were recorded while energy was swept at 0.25 eV/sec by oscillation of a Faraday cup (FC) back and forth across the beam position. A very important factor in the long data-accumulation times was an x-ray-corrected total system pressure less than 1×10^{-11} Torr. Once the sample was cooled to < 200 K within ten minutes of a flash to > 2500 K, the half-order spectra would remain unchanged for 2 hours or

more.

Figure 1 shows a schematic of those LEED beams at normal incidence which could be monitored with the FC, obtained at crystal temperatures between 170 and 190 K. The mirror lines are indicated by dashed lines and by labeling the spots of a particular $[h/2, k/2]$ or $(\pm h/2, \pm k/2)$, $(\pm k/2, \pm h/2)$, etc., set of beams with + and - according to which one of the two spectral types their $I-V$ curves belong to.

Figure 2 shows five of the eight $[\frac{5}{2}, \frac{3}{2}]$ beam spectra, which clearly display the $2mm$ point-group symmetry. The close agreement of the $(\frac{5}{2}, \frac{3}{2})$, $(\frac{3}{2}, \frac{5}{2})$, and $(\frac{5}{2}, \frac{3}{2})$ spectra attests to $\theta = 0^\circ$. The start of the $(\frac{5}{2}, \frac{3}{2})$ beam is missing because of the blockage by the crystal holder. The $[\frac{5}{2}, \frac{1}{2}]$ and $[\frac{3}{2}, \frac{1}{2}]$ beam sets show similar subtle but completely reproducible mirror-plane effects.

Figure 3 shows examples of the two spectral types, differing only in absolute intensity by a nearly constant factor for the $[\frac{1}{2}, \frac{1}{2}]$ and $[\frac{5}{2}, \frac{5}{2}]$ beam sets. The $[\frac{3}{2}, \frac{3}{2}]$ show the same effect over a larger energy range. The $(-h/2, h/2)$ spectra

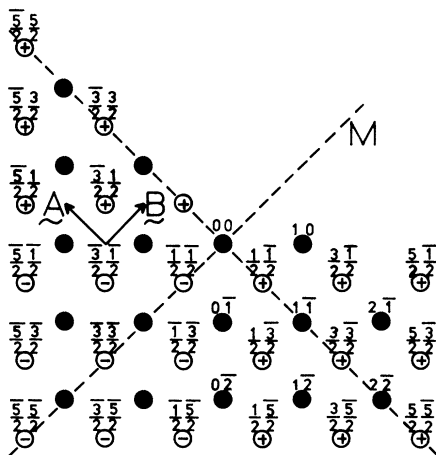


FIG. 1. Schematic of the LEED pattern labeling the beams measured with the FC. Within each set of beams, i.e., $(\pm h/2, \pm k/2)$ and $(\pm k/2, \pm h/2)$, etc., the individual beams are distinguished by + and - according to which spectral type they belong to as generated by the mirror planes (dashed lines). The primitive reciprocal unit mesh is defined by \vec{A} and \vec{B} .

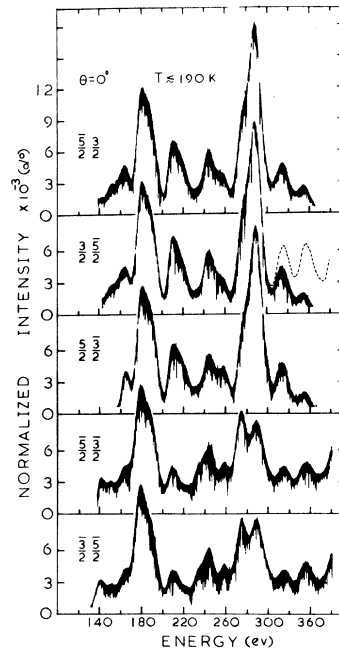


FIG. 2. Direct reproduction of five of the eight $[\frac{5}{2}, \frac{3}{2}]$ beam spectra displaying the subtle $2mm$ point-group symmetry characteristic of all the half-order beam sets and the $[21]$ beams when the $(\sqrt{2} \times \sqrt{2})R45^\circ$ forms. The envelope of vertical lines forming the $I-V$ curves result when the FC is swept back and forth across the moving beam position. These spectra were very reproducible but the dashed curve shows the intensities obtained on three occasions without any satisfactory explanation why the change occurred.

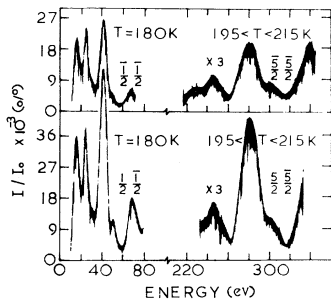


FIG. 3. Example of the two spectral types, differing only in absolute intensity by a nearly constant factor for the $[h/2, h/2]$ beam sets. This effect can be explained by the preferred orienting of $(\sqrt{2} \times \sqrt{2})R45^\circ$ domains, each having a $p2mg$ space-group symmetry. Deviations from normal incidence as small as $\frac{1}{4}^\circ$ can account for the larger relative intensity of the 41.5-eV peak in the $(\frac{1}{2}, -\frac{1}{2})$ spectrum.

(not shown) in each case have the same absolute intensities as the $(h/2, -h/2)$ beams. These differences were visually apparent in the LEED pattern as well. The larger relative intensity of the 41.5-eV peak in the $(\frac{1}{2}, -\frac{1}{2})$ spectrum is believed to be due to deviations as small as $\frac{1}{4}^\circ$ from exactly normal incidence. The same spectra taken on other days showed just the reverse effect.

Observation of a lower point-group symmetry in the LEED pattern than that possessed by the substrate can only be the result of unequal numbers of equivalent domains. Such an effect is well documented on cleaved Ge(111)(2×1) and Si(111)(2×1) structures,^{6,7} which show mixtures of the three possible (2×1) domain orientations, with the preferred domain orientation determined by which $\langle 211 \rangle$ direction lay closest to the cleavage direction. Other examples exist; however, to our knowledge this is the first example of a domain orientation preference in a structure displaying $(r \times r)R\theta^\circ$ translational symmetry.

As Fingerland⁸ points out, the surface-structure space group must be a subgroup of the substrate, which for $W\{001\}$ is $p4mm$. The observed $2mm$ point-group symmetry limits this to four possibilities: $p2mm$, $p2mg$, $p2gg$, and $c2mm$.⁹ Use of the fact that differences in only absolute intensity occur in the half-order diagonal beams, as illustrated in Fig. 3, allows a unique choice from these four space groups. In this regard it is important to note another fact of the diffraction pattern: No beam-broadening, streaking, or splitting, as results from interference among antiphase domains,¹⁰ was observed in the half-order beams. Hence, the various

$(\sqrt{2} \times \sqrt{2})R45^\circ$ domains were scattering incoherently and the measured intensity in a given beam was just the superposition of intensities from the individual domains. On any given step plane of the surface, then, there are four possible $2mm$ domain registries. Any two are related by either a translation by a substrate unit mesh vector, or a rotation through 90° . If n_1 , n_2 , n_3 , and n_4 are the respective numbers of such incoherently scattering domains, assumed for simplicity to have the same average size, by superposition of intensities, the measured intensity versus energy of the (hk) beam (choosing the primitive reciprocal unit mesh of one of the domains to index the measured beams so that the extra-order beams now have odd-integer indices) is $I(hk) = (n_1 + n_3)I_1(hk) + (n_2 + n_4)I_2(k\bar{h})$, where $I_i(hk)$ is the intensity scattered from the average domain type i into its (hk) beam. The relationship between the absolute intensities of the $(h0)$ and $(0h)$ beams (the diagonal half-order beams when using the substrate reciprocal mesh for indexing), shown in Fig. 3, is expressed as $I(h0) = fI(0h)$ for h an odd integer and f a constant not equal to 1. Hence

$$f = \frac{(n_1 + n_3)I_1(h0) + (n_2 + n_4)I_2(0h)}{(n_1 + n_3)I_1(0h) + (n_2 + n_4)I_2(h0)} \neq 1. \quad (1)$$

Since $2mm$ symmetry means $I_i(hk) \neq I_i(k\bar{h})$ unless $|h| = |k|$, but $I_i(hk) = I_j(hk)$, there are only two ways that (1) can be satisfied with f a constant: either $I_1(0h) = 0$ and $I_2(0h) = 0$ or $I_1(h0) = 0$ and $I_2(k0) = 0$, making f equal to $(n_1 + n_3)/(n_2 + n_4)$ or its reciprocal. The observed effect shown in Fig. 3 demands that the odd-integer $(h0)$ beams parallel to one reciprocal primitive unit mesh vector, say \vec{A} , vanish but not the $(0h)$ beams parallel to \vec{B} .

Holland and Woodruff¹¹ have presented equations which allow the determination of the consequence of crystal symmetry at any incidence angle, and from which the conditions for systematic absences can be derived from a completely general scattering formalism. If \vec{k} and \vec{k}' are the incident and reflected wave vectors, and T the transition operator, then the scattering amplitude is determined by the matrix element $\langle k' | T | k \rangle$. For the special case of the glide plane parallel to \vec{a} and a beam on the glide line, it readily follows that $\langle \vec{k}' | T | \vec{k} \rangle = e^{i\pi h} \langle \vec{k}' | T | \vec{k} \rangle$. Hence, either $\langle \vec{k}' | T | \vec{k} \rangle = 0$ or h is even, i.e., the $(h0)$ beams vanish for h odd. Equally important, if the incident wave vector lies in a plane parallel to the glide plane, as is trivially true at normal incidence, it follows¹¹ that the glide plane still gives reflection symmetry for intensities (though not

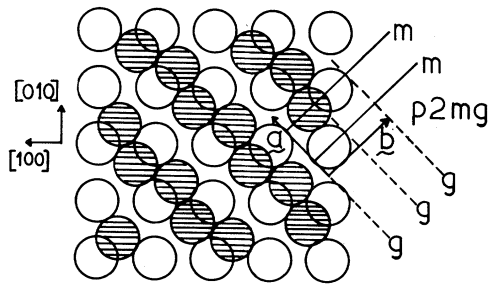


FIG. 4. A top-layer rearrangement ball model for a $(\sqrt{2} \times \sqrt{2}) R45^\circ$ domain having $p2mg$ symmetry. For a single-layer rearrangement model, this structure appears to be unique. The primitive unit mesh is defined by \vec{a} and \vec{b} and its symmetry elements are indicated: g = glide plane, m = mirror plane.

amplitudes) as we must have for $2mm$ symmetry in the added intensities from all the domains.

Thus the data of Figs. 2 and 3 can be completely explained by the preferential orienting of $(\sqrt{2} \times \sqrt{2}) R45^\circ$ domains having glide planes parallel to \vec{b} and mirror planes parallel to \vec{a} , the primitive unit mesh vectors, conditions satisfied only by the $p2mg$ two-dimensional space group.

Only one structure could be found having this symmetry for a rearrangement restricted to a single layer. This is illustrated in Fig. 4. The top-layer atoms have moved along the diagonals of the substrate mesh (by an indeterminate amount), to form zigzag rows parallel to the $[110]$ direction. The gentle rearrangement of surface tungsten atoms in this structure is also consistent with the relatively low temperature (370 K) at which the surface reverts to a (1×1) structure.^{1,2} Dynamical LEED calculations are presently being carried out to test this model as well as other $(\sqrt{2} \times \sqrt{2}) R45^\circ$ structures to determine the sensitivity of the calculations to such gentle rearrangements.

Much consideration has been given to other possible reasons for the effect seen in Fig. 3, but it would seem no ordered or random surface defect, artifact, etc., could affect the half-order beams without similarly affecting the integral-order beams on the same diagonal. The $[11]$ beams show identical absolute intensities. Even more convincing, this glide-plane effect is absent from the $(\sqrt{2} \times \sqrt{2}) R45^\circ$ -H₂ structure,⁵ produced by hydrogen adsorption on the same sample without any intermediate treatment.

Also of interest is why we were fortunate enough to have the domain degeneracy removed, giving a preferred orientation and allowing the

full symmetry of an individual domain to be seen. It seems certain to be a boundary effect. The integral-order spots showed a slight, unresolved splitting, due to steps, just sufficient to calculate¹² a mean terrace width of $\sim 85 \text{ \AA}$ and minimum step height. Since the step edges were not always exactly parallel to the $[010]$ direction, there is some evidence to suggest that the preferred domains are those whose zigzag rows lie most nearly parallel to the step edges. But as for the Ge(111)⁷ case, no splitting of the half-order beam was ever detected at any energy regardless of the degree of integral-order beam splitting, and the effect of Fig. 3 persisted when the step edges were exactly along the $[010]$ direction. Since the half-order beams showed no step interference effects, nor out-of-phase domain interference effects, we are led to believe with the present evidence that the $(\sqrt{2} \times \sqrt{2}) R45^\circ$ domains occupy the terrace centers, surrounded by (1×1) zones which contain the step edges and have a width on the order of the beam coherence width.

A structure (Fig. 4) has been proposed for the $W\{001\}: (\sqrt{2} \times \sqrt{2}) R45^\circ p2mg$, for which it is hoped that the actual displacement magnitudes can be determined by dynamical LEED calculations. The driving mechanism for this low-temperature phase is yet to be determined.

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