PHYSICAL REVIEW B VOLUME 60, NUMBER 3 15 JULY 1999-I

Surface roughness and LEED crystallography: Analysis of flat and vicinal W(110)

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(Received 28 August 1998; revised manuscript received 22 December 1998)

Low-energy electron diffraction intensity vs voltage (LEED I-V) measurements and analysis are used to determine the multilayer surface relaxation of W(110). Measurements and analysis are presented for both flat and vicinal surfaces, demonstrating that surface roughness leads to only small errors in LEED structure determinations. Flat, clean W(110) exhibits first-(d_{12}) and second-(d_{23}) layer relaxations of $-3.0\pm1.3\%$ and $+0.2\pm1.3\%$, respectively, relative to the bulk lattice spacing $d_0=2.237$ Å. This experimentally determined surface relaxation of W(110) is compatible with a recent combined density-functional theory calculation and LEED study [M. Arnold, G. Hupfauer, P. Bayer, L. Hammer, K. Heinz, B. Kohler, and M. Scheffler, Surf. Sci. **382**, 288 (1997)]. Surface roughness (in the present case, uniform atomic height steps) is found to produce a small apparent increase in the measured value of d_{12} when determined using standard (flat surface) LEED I-V methodology. However, for low step densities (<20 atoms/step) the apparent change in d_{12} is small compared to other sources of error, so it is unlikely that surface roughness is a significant source of error in LEED structure determinations. [S0163-1829(99)00327-6]

I. INTRODUCTION

Recent interest in the structure of surfaces[1,2] has focused, in part, on what appear to be systematic discrepancies[3] between first-principles calculations and experimental determinations of the first-layer relaxation at selected crystal faces of reactive transition metals: Ti(0001), Zr(0001), Ru(0001), Mo(110), W(110), and Rh(001). The magnitude of the discrepancies, based on available experimental results, generally exceeds the accepted accuracy of both the experimental techniques and the theoretical calculations.[3] Specifically, the calculations systematically predict top-layer relaxations of these surfaces that are a factor of 2-5 larger than available experimental values. It is not clear whether these disagreements are a consequence of errors in experimental or theoretical methodology, or both. Large variations of d_{12} are apparent when comparing separately the experimental and theoretical values for a given surface [refer to Table I for W(110) and the corresponding Table I in Ref. 2 for Rh(001)]. However, in spite of the scatter in theoretical and experimental results considered separately, the systematic discrepancies, noted and discussed by Feibelman,[3] appear to be real based on the presently available experimental and theoretical work.

Resolving the origin of these discrepancies between measured and calculated surface relaxations is important for several reasons. According to conventional wisdom, this classic surface structure problem has been solved: in many cases where low-energy electron diffraction (LEED) analysis has yielded surface structural parameters with good confidence levels (r factors), first-principles local-density-approximation calculations produce relaxations in excellent agreement. One would certainly like to know if the apparent discrepancies for reactive transition metals can be traced to surface contamination (hydrogen, specifically) or defects such as surface

TABLE I. First- and second-layer surface relaxation of W(110). Quoted values are in percent of bulk interlayer spacing $d_0=2.237$ Å.

	$\Delta d_{12}/d_0$ (%)	$\Delta d_{23}/d_0$ (%)
Experiment		
Buchholz and Lagally[a]	0.0 ± 3	
Van Hove and Tong[b]	0.0	
Smith *et al.*[c]	<2	
Kim *et al.*[d]	0.0 ± 1.0	
Arnold *et al.*[e]	-3.1 ± 0.6	0.0 ± 0.9
Present work	-3.0 ± 1.3	$+0.2\pm1.3$
Theory		
Luo and Legrand[f]	-1.4	-0.4
Rodriguez *et al.*[g]	-2.1	$+0.7$
Xu and Adams[h]	-5.0	$+4.6$
Arnold *et al.*[e]	-3.6	$+0.2$

[a] LEED Ref. 8.
[b] LEED Ref. 9.
[c] High energy ion scattering, Ref. 10.
[d] Photoelectron diffraction, Ref. 11.
[e] LEED and nine-layer DFT calculation, Ref. 1.
[f] Tight binding approximation, Ref. 12.
[g] Reference 13.
[h] Tight binding approximation, Ref. 14.

0163-1829/99/60(3)/1975(7)/$15.00

roughness. Resolving the discrepancies may also help to clarify our understanding of the basic mechanism responsible for relaxation at metal surfaces. Consistently small contractions (as currently observed experimentally for the subject metals) tend to support the ''charge smoothing'' picture of Finnis and Heine,[4] in which electrons above surface atoms tend to fill the spaces between them. This redistribution of charge at the surface (Smoluchowski charge smoothing[5]) leads to the electrostatic interactions that induce surface relaxation. Large relaxations for close-packed or quasi-close-packed surfaces, such as those predicted by recent LDA calculations,[6,7] favor the ''promotion-hybridization'' picture put forth by Feibelman.[6] In this interpretation of surface relaxation, the correlation between dimer bond lengths and surface relaxations is noted, which leads to chemical arguments that may explain trends in surface relaxation. General trends in surface relaxation may indicate whether surface relaxation is dominated by lowering of the valence electron kinetic energy at a surface, or by the rehybridization of surface chemical bonds.

A survey of the literature representing experimental structure studies of the subject metal surfaces reveals that many of the experiments based on low-energy electron diffraction intensity vs voltage (LEED I-V) were carried out over ten years ago. Examination of Table I covering structural data for W(110) illustrates the trend in experimentally[1,8–11] and theoretically[1,12–14] determined values of d_{12}: early LEED experiments and our own recent photoelectron diffraction analysis of W(110) concluded that the surface layer terminates in essentially an ideal bulk crystal geometry $(\Delta d_{12}/d_0 \sim 0\%)$. Early theoretical work obtained values for $\Delta d_{12}/d_0$ ranging from -1.4% to -5%. The range of theoretically determined values of d_{12}, and the trend in differences between theoretical and experimental values illustrated in Table I, is typical of the other subject metal surfaces. The recent work of Arnold *et al.*[1] (refer to Table I, this work), in which state-of-the-art density-functional-theory (DFT) calculations are compared with new LEED results, appears to have resolved the dilemma for the W(110) surface. The new calculation again predicts a significant relaxation, consistent with prior theoretical results. The new LEED experiment, in contrast to prior experimental work that yielded essentially a bulk (unrelaxed) termination, also obtains a substantial surface relaxation.

A similar calculation by the same group[15] yields a surface relaxation of -1.4% for Rh(001) at 300 K, including a substantial correction resulting from vibrational excitations. Our LEED results[2] for Rh(001) yielded an outward expansion of $+1.0\pm0.5\%$. Prior experimental results for Rh(001) are: Watson *et al.*,[16] $0.0\pm3.0\%$; Oed *et al.*,[17] $+0.5\pm1.0\%$; Begley *et al.*,[18] $-1.2\pm1.6\%$; and Prince *et al.*,[19] $-1.1\pm3.6\%$. Because of this persistent discrepancy, we have obtained a different Rh(001) crystal and have repeated our LEED I-V measurements and analysis using the methodology described in this paper (SATLEED code with 13 relativistic phase shifts). The preliminary result for data taken at 350 K is: $\Delta d_{12}/d_0 = -1.4\pm1.4\%$.[20] This result is in better agreement with the theoretical result of Cho and Scheffler,[15] as well as the most recent experimental values.[18,19] It is not yet clear what accounts for the discrepancy between our new results and our previous results. Any difference in data sets and analysis appear to be very subtle; additional effort is being directed toward resolving this difference.

The present paper continues to explore the surface relaxations of the reactive transition metal surfaces identified by Feibelman. In our previous LEED study of Rh(001), we explicitly addressed the ''hydrogen contamination'' issue in relation to surface relaxation measurements. In addition, we obtained exactly the same surface structural parameters by analyzing several LEED I-V data sets using different LEED structure search codes and *r* factors. In the present LEED study of W(110), our objective was to obtain independent values of d_{12} and d_{23}, in an attempt to determine which of the various existing experimental results for W(110) is valid. The present study also addresses relevant issues that pertain to the accuracy of a LEED surface structure determination. Specifically, special attention is given to residual hydrogen contamination, issues associated with surface roughness, and the energy range of the data set.

Our LEED study of $p(1\times1)$ H on Rh(001)[2]—as well as the corresponding study by Arnold *et al.*[1] of $p(1\times1)$ H on W(110)—demonstrates that surface hydrogen substantially alters the multilayer relaxation of a metal surface. The change in d_{12} induced by a full monolayer coverage can be used to estimate errors resulting from the low coverages of residual hydrogen or other surface contamination that inevitably form during LEED I-V measurements. Based on experience gained during our study of $p(1\times1)$ H on Rh(001)[2], on our electron-energy loss spectroscopy (EELS) studies of hydrogen uptake on W(110), and on the experimental conditions maintained during LEED I-V data acquisition for W(110), discussed later, we judge that errors in d_{12} resulting from hydrogen or other impurity atoms are negligible in the present study. Arnold *et al.*[1] carried out extensive LEED I-V analysis of $p(1\times1)$ H on W(110) in conjunction with their analysis of the clean surface. The excellent agreement (discussed later) between LEED I-V spectra and structural results obtained in the present work with that of Arnold *et al.* is another indication that hydrogen or other surface contamination has not affected the structural results.

In addition to established sources of error in LEED analysis resulting from contaminants, specifically surface hydrogen, surface roughness has been identified as a possible source of error in LEED structure determinations.[3] Strain fields due to lattice defects, including surface steps, decay over distances of several unit cells. It is possible that defect-driven strains at high-enough density can modify surface relaxation. In addition, it is well established that open surfaces exhibit large relaxations compared to close-packed and quasi-close-packed surfaces.[21] Based on this trend, one might expect atoms near step edges at a rough surface to exhibit larger relaxations, due to lower coordinations, than atoms with ideal coordinations. A LEED experiment averages over a large region of the surface, so for high-enough step density, this could lead to a decrease in the measured value of d_{12}. One also worries that errors are introduced into the analysis when a rough or vicinal surface is analyzed with a flat surface model. When this is done, the phase shifts between adjacent terraces are neglected in the dynamical LEED analysis, and it is not intuitively obvious what effect this has on the structure search results.

One of the purposes of the present study is to characterize how surface roughness affects LEED I-V experiments and analysis. It is well known that surface roughness produces broadening or splitting of diffracted electron beams, and increases diffuse intensity. The present study demonstrates that surface roughness modifies LEED I-V spectra, leading to slightly different structural parameters. Prior analysis of a model vicinal surface, with step widths smaller than the electron coherence length, has shown that such a step distribution reduces Bragg peak intensities, and shifts the intensity profiles to higher energies.[22] The experimental technology for obtaining LEED I-V data at the high angular resolution required to characterize beam splitting and broadening from a vicinal surface exists. However, LEED codes capable of analyzing such data efficiently have not yet been developed. Therefore, a rigorous analysis of surface step-induced structure is not feasible at present. Nevertheless, by applying standard LEED I-V methodology to a series of surfaces having known step density, it is possible to assess empirically the degree to which surface roughness affects the accuracy of LEED structure analyses.

II. EXPERIMENTAL PROCEDURES

The experimental apparatus used to carry out these measurements has been described in Ref. 2. The W(110) crystal was spark cut from a tungsten boule after alignment using x-ray Laue techniques. The lens-shaped crystal surface was prepared by mechanical polishing to have a flat region of [110] alignment near the center of the $14\times10\times1$-mm sample, and convex surface profiles (in all directions) extending to the edges. The step-density ranges from a low value near the sample center (limited by the intrinsic roughness of the sample) to a value of approximately one step/20 Å (5° vicinal) along the $[1\bar{1}0]$ surface direction. The minimum step density near the center is too small to be resolved by the conventional Varian four-grid LEED optics (resolving power estimated to be ~one step/100 Å). Away from the flat region, the step density can be accurately measured by analysis of beam broadening and splitting.

In situ sample preparation consisted of annealing the sample at 1600 K in oxygen to deplete near-surface carbon, followed by repeated cycles of glancing incidence sputtering (5–10 mA/cm^2 at 2×10^{-4} torr Ne) and annealing. Any residual oxygen detected after sputtering and annealing was removed by flashing the sample to 2300 K for a few seconds. This procedure resulted in a surface free of contaminants as monitored with Auger electron spectroscopy. Electron-energy loss spectroscopy (EELS) studies of hydrogen uptake at W(110) were carried out initially (similar to those described in Ref. 2) to verify that the LEED experiments would not be affected by surface hydrogen contamination.

LEED I-V data sets were acquired after symmetrizing conjugate (symmetry-degenerate) beams in the usual manner: the orientation of the sample was adjusted so that all conjugate beams had the same intensity. This procedure insures normal incidence of the electron beam. For data taken on vicinal regions of the sample, conjugate beams were first symmetrized on the flat region, and then the sample was translated perpendicular to the incident beam to achieve the desired step density. Thus, the beam was at normal incidence to the terraces in all cases, although not to the macroscopic surface for vicinal regions.

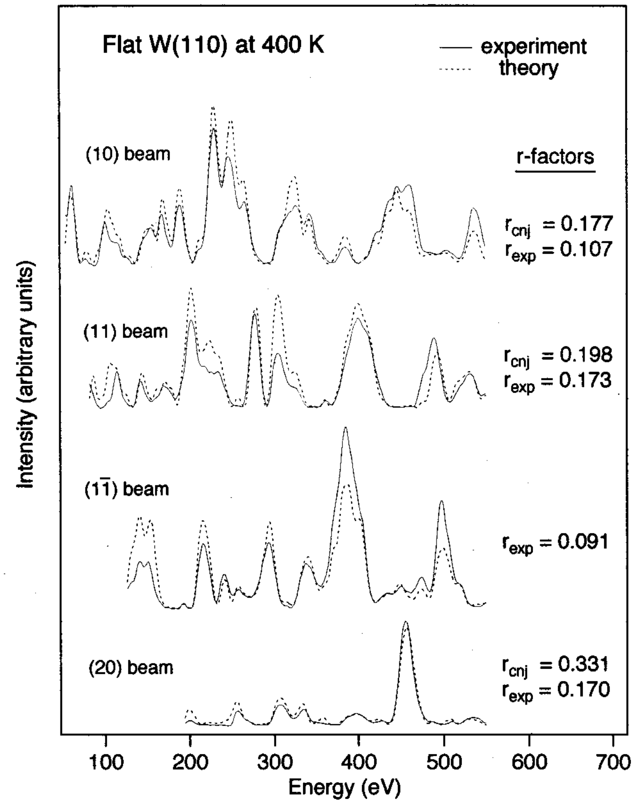

FIG. 1. Measured and calculated LEED I-V spectra for flat W(110) at 400 K. Two r factors are indicated for each conjugate beam, which compare various *experimental* spectra. The r_{cnj} are the averages of the Pendry r factors between experimental conjugate beams within each independent data set. The r_{exp} are the averages of the Pendry r factors between independent conjugate-beam-averaged data sets. The r factors characterizing theory-experiment comparisons are presented in Table II.

Vicinal surface data sets were taken for surfaces with steps along the $[1\bar{1}0]$ direction. The step density was calculated directly from the broadening or splitting observed in the diffracted beams. The incident electron beam at the sample has a finite diameter of about 0.5 mm. This fact, coupled with the continuous step gradient that resulted from our sample preparation procedure, means that each of our LEED I-V data sets from flat and vicinal W(110) surfaces represents an effective average over a small range of step densities. The step density increased uniformly with distance from the flat region near the center. The experiments yielded no evidence of step bunching or roughening resulting from the surface cleaning procedures. Therefore, meaningful and accurate average step densities could be inferred from the LEED spot profiles.

III. LEED DATA AND ANALYSIS

Figure 1 displays a set of conjugate-beam-averaged LEED I-V data for ‘‘flat’’ W(110) at 400 K. Based on LEED beam spot profiles for this region of the surface (which we judge to be instrument resolution limited) the average step density is less than one step/100 Å. The r factors indicated in

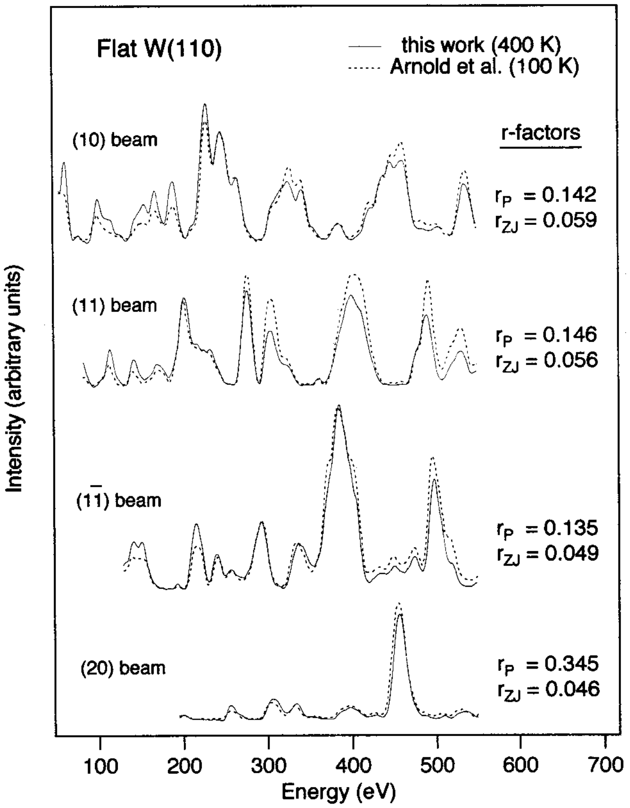

FIG. 2. Comparison of two independently measured sets of LEED I-V data for W(110). The solid line represents this work (400 K), while the dashed line is taken from the work of Arnold *et al.* (100 K) (Ref. 1). The *r* factors (Pendry and Zanazzi-Jona) characterize the agreement between the two data sets.

the figure for each beam compare experimental conjugate beams, and characterize the consistency of conjugate beams within each conjugate-beam-averaged I-V curve. Superimposed on the experimental I-V curves are the optimized calculated I-V curves, to be discussed. The *r* factors characterizing theory-experiment comparisons are also discussed later.

In our published[2] LEED study of Rh(001), we carried out an exercise to determine the compatibility of data sets obtained by different groups. This can be considered an extension of the 1980 international LEED project[23,24] on Cu(001) designed to assess the intrinsic accuracy of LEED I-V technology (at that time). For Rh(001), an *r* factor comparison of data sets found values of $r_{ZJ}\sim0.05$ (Zanazzi-Jona *r* factor) and $r_x\sim0.02-0.06$ (x-ray *r* factor). These are very good *r* factors, indicating excellent agreement between independent data sets measured by different groups. A similar exercise was carried out comparing our LEED I-V data for W(110) with that of Arnold *et al.*[1] The results are shown in Fig. 2. Qualitatively, the two data sets appear quite compatible, and again, low-*r* factors ($r_{ZJ}\sim0.05$, $r_P\sim0.25$) indicate a high degree of correlation.

The Barbieri/Van Hove SATLEED code,[25] which incorporates standard *r*-factor analysis, was used to calculate theoretical I-V spectra. The calculations used 13 relativistic phase shifts obtained from the Barbieri/Van Hove phase shift code.[26] Thermal corrections were included using a bulk Debye temperature for tungsten $\Theta_{DB}=380\,\mathrm{K}$, as used in prior LEED studies.[1,9] The best value for the surface Debye temperature was found to be $\Theta_{DS}=300\,\mathrm{K}$. Surface atomic vibrational amplitudes were taken to be isotropic with respect to the parallel and perpendicular surface directions. The imaginary part of the inner potential V_{oi} was fixed at -5.0 eV. The real part of the inner potential V_{or} was allowed to vary as part of the structure search for each data set: optimum values ranged from 2.8 to 4.5 eV. Based on the null result obtained by Arnold *et al.*[1] in searching for evidence of a top-layer registry shift, we restricted our structure search to multilayer relaxation of surface atoms assumed to be in registry along the [110] (surface normal) direction.

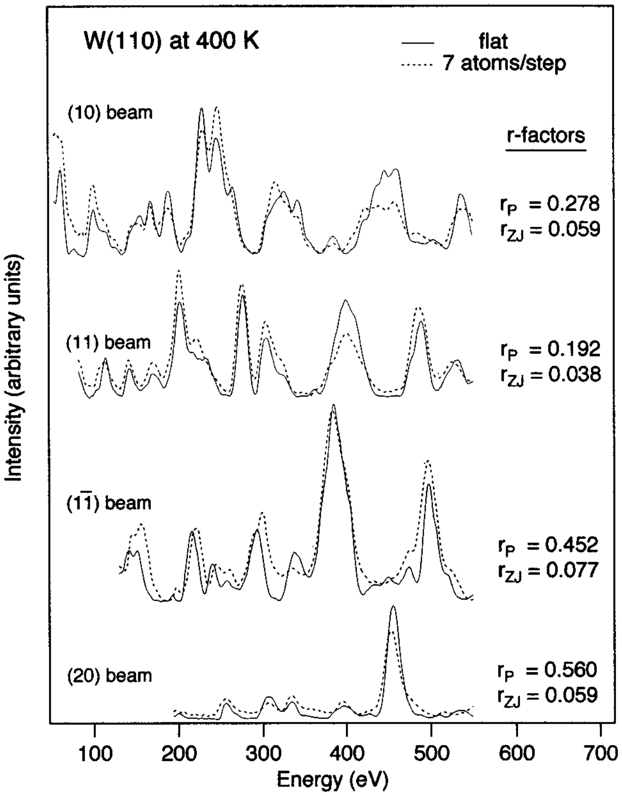

FIG. 3. Comparison of experimental LEED I-V spectra for flat and stepped W(110) at 400 K. The *r* factors (Pendry and Zanazzi-Jona) characterize the level of agreement between the two data sets.

Figure 3 compares two data sets: one obtained from the region of the surface judged to have the lowest step density, and a second from a region where the LEED spot splitting indicated a step density corresponding to 7 atoms/step along the $[1\bar{1}0]$ direction. The intensities displayed for the vicinal surface were obtained by integrating the intensities of the split beams. Otherwise, data sets from flat and vicinal surfaces were processed identically. LEED I-V data sets were measured and analyzed for four different step densities corresponding to average terrace widths of 7, 10, 15, and 20 atoms. Table II presents the results of LEED structure analysis of the flat and vicinal W(110) surfaces. The same set of optimized nonstructural parameters obtained for the flat surface analysis was used for analyzing the vicinal surface data.

IV. DISCUSSION

Our LEED results for the surface relaxation of W(110) corroborate the recent work of Arnold *et al.*[1] (see Tables I

TABLE II. Summary of structure search results for flat and vicinal W(110) surfaces.

Data set	r_p	$\Delta d_{12}/d_0$ (%)	$\Delta d_{23}/d_0$ (%)	$\Delta d_{34}/d_0$ (%)	Uncertainty (%)
Flat	0.202	−3.0	+0.2	−1.0	±1.3
Atoms/step					
20	0.305	−2.7	+0.0	−0.5	±2.2
15	0.300	−2.5	−0.1	−0.7	±2.2
10	0.389	−2.3	−0.3	−0.5	±2.7
7	0.428	−1.9	−0.6	−1.0	±2.7

and II). The Pendry[27] r factor r_P was used as the criterion for theory-experiment comparison in our structure searches. The limits of statistical error (discussed in Ref. 27) for the structural parameters determined using this criterion were estimated by its variance $\mathrm{var}(r_P)=r_{min}\sqrt{8V_{oi}/\Delta E}$. Based on the minimum values of r_P, we obtain from our structure search for flat W(110) $\Delta d_{12}/d_0=-3.0\pm1.3\%$ and $\Delta d_{23}/d_0=+0.2\pm1.3\%$.

The structural parameters for flat W(110) obtained from our LEED I-V analysis are essentially identical to those obtained by Arnold *et al.*[1] (Table I), but differ substantially from those of earlier LEED and photoelectron diffraction studies. One feature of the prior work that sets it apart from our present LEED study and that of Arnold *et al.*, is the size of the data set analyzed. The present structure analysis is based on LEED I-V spectra from four inequivalent beams to an energy of 550 eV, corresponding to a data set covering an equivalent range of about 1800 eV. The early LEED study[9] of W(110) is based on experimental I-V curves for inequivalent beams extending to just above 200 eV, covering a cumulative energy range of about 600 eV. The photoelectron diffraction results[11] were based on an even smaller data set, of the order of 100 eV, except some angular dependent data were also included in the analysis, which probably doubled the effective data-set size.

In order to explore the consequences of analyzing a smaller data set on the accuracy of structural results obtained from a LEED I-V experiment, and to improve our intuitive understanding of how various r factors affect structural results, we carried out a series of structure searches based on subsets of the full data set. The Barbieri/Van Hove SATLEED code allows the user to apply any one of ten r factors to the theory-experiment comparison, or to create a hybrid r factor by giving arbitrary weighting factors to the individual r factors. We ran three sets of structure searches using r_P and r_{ZJ} independently, and r_P and r_{ZJ} in combination (with equal weighting factors). The results are presented in Fig. 4. The upper panel shows the variation of $\Delta d_{12}/d_0$ obtained from each of the three r factors applied to data sets that are decreased in 5 eV increments from a full set (550 eV energy cutoff, corresponding to an energy range of ~1800 eV) to an energy cutoff of 100 eV. The lower panel plots the corresponding evolution of the r factors. Error bars on $\Delta d_{12}/d_0$ obtained from the Pendry r factor are shown for a few representative values of energy cutoff.

The trends apparent from data presented in Fig. 4 are reasonable. The value of $\Delta d_{12}/d_0$ obtained from each of the r factors converges and the value of each r factor decreases as the energy cutoff (size of the data set) is increased. The Zannazi-Jona r factor consistently produces a slightly larger value of d_{12} than the Pendry r factor, but the difference is small compared to the error bars based on the variance of r_P. It is reasonable that the scatter of $\Delta d_{12}/d_0$ increases as the cumulative energy range is reduced below about 800 eV. However, it is interesting that the values of d_{12} determined from data sets with cumulative energy ranges below 800 eV tend to be nearer the bulk value. This trend may contribute to the differences in experimentally determined surface structure parameters apparent from Table I.

Analysis of vicinal surface LEED I-V data yields a systematic trend in structural values apparent from Table II. Using the same nonstructural parameters (phase shifts, Debye temperature, real and imaginary parts of the inner potential, etc.), and using r_P to carry out the structure search, the values of d_{12} that minimize r_P increase monotonically to-

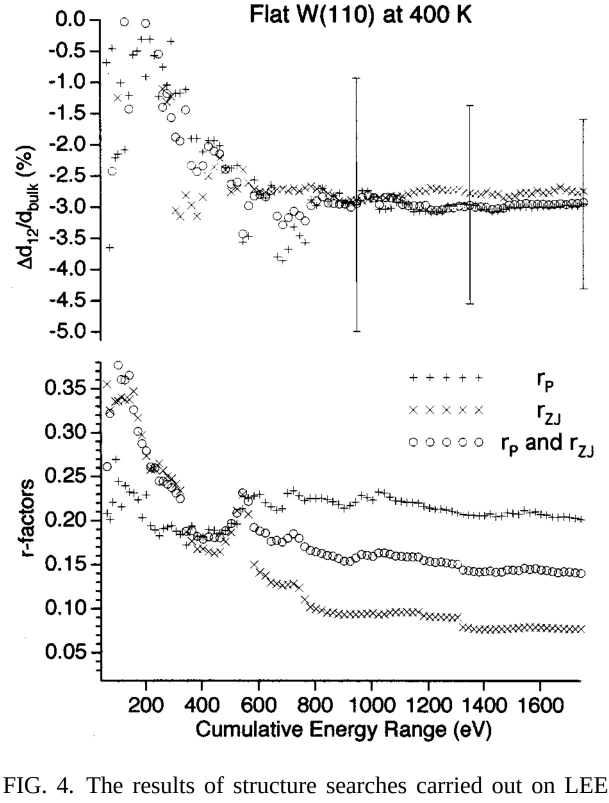

FIG. 4. The results of structure searches carried out on LEED I-V data from flat W(110) at 400 K using the Barbieri/Van Hove SATLEED code. Subsets of the data were analyzed by varying the energy cutoff from 100 to 550 eV. The upper panel shows the results for d_{12} vs cumulative energy range (summed over all inequivalent beams), while the lower panel displays the evolution of the r factors (Pendry, Zanazzi-Jona, and an equal weighting of the two). The error bars in the upper panel are based on the variance of the Pendry r factors.

ward the bulk value as the step density increases. The sensitivity of structural parameters to step density is not extremely high. The estimated accuracy of the value of d_{12} for the flat surface is $d_{12}=2.169\pm0.02$ Å. The variation of d_{12} obtained from analysis of a flat and a 20 atom-per-terrace sample is (d_{12} vicinal$-d_{12}$ flat)$=2.175$ Å-2.169 Å$=0.006$ Å, over a factor of three smaller than the intrinsic accuracy of the structure determination methodology based on the variance in r_P.

We note that the apparent increase in d_{12} resulting from the analysis of a vicinal surface does not necessarily imply that the steps actually induce a change in the surface relaxation. The apparent increase in d_{12} is more legitimately viewed as an error produced by the methodology when an inappropriate (flat surface) model is applied to a surface having roughness. While it is certainly possible that steps induce significant changes in surface structure, it is not feasible with present computational resources to carry out LEED calculations for the large unit cells necessary to describe vicinal surfaces. Furthermore, based on the charge-smoothing arguments that apparently explain the trend of large relaxations for more open surfaces, one would expect surface roughness to lead to a decrease in the average value of d_{12}, rather than an increase.

We emphasize that we have applied a flat surface structural model (in the SATLEED codes) to surfaces known to have steps. Therefore, it would be inappropriate to attempt to extract meaningful information about step-induced structural changes from our analysis of vicinal surfaces. The important point is that the procedure used here permits accurate characterization of the loss in accuracy that results from analyzing experimental data from a rough or vicinal surface with a flat surface model. The procedure we have employed is not capable of distinguishing between real step-induced structural changes and errors that result from applying a flat surface model to vicinal surface data.

Typical commercial display LEED systems have instrumental transfer widths of 100–150 Å, and are easily capable of distinguishing between a ''flat'' sample and one with steps (or comparable surface island structure) having 20 or fewer atoms per step. With a good ''flat'' reference crystal, Si(100) 2×1 for example, which yields spot profiles that characterize the instrumental response, a semiquantitative estimate of the surface quality is directly apparent from the LEED pattern to a sensitivity approaching the resolving limit of the system. Based on the results presented in Table II, extrapolation of the errors in d_{12} caused by steps suggests that these errors are negligible for a surface judged as ''flat'' based on an excellent quality LEED pattern from a good commercial LEED instrument.

V. CONCLUSIONS

The multilayer relaxation of W(110) determined by our LEED I-V analysis is in very good agreement with the most recent DFT calculations, and with a recent independent LEED analysis. The flat, hydrogen-free W(110) surface exhibits a first-layer relaxation of $\Delta d_{12}/d_0=-3.0\pm1.3\%$, and a slight second-layer outward relaxation of $\Delta d_{23}/d_0=+0.2\pm1.3\%$. This result, a rather large contraction for a quasi-close-packed transition-metal surface, lends support to the promotion-hybridization picture of surface relaxation put forth by Feibelman.[6]

Surface roughness has been suggested as a possible underlying cause of the systematic discrepancies between surface structure determined separately from *ab initio* calculations and from LEED I-V measurements. We have applied the standard flat surface LEED I-V methodology to vicinal W(110) surfaces with uniform step densities. This analysis permits an empirical assessment of the sensitivity of LEED structure determinations to surface roughness, or to vicinalities resulting from a misaligned crystal. The observed systematic variation of d_{12} as a function of step density permits extrapolation of the surface-roughness-induced error to the roughness limit detectable by a standard commercial LEED instrument. This extrapolation indicates that surface step density or roughness at this limit (approximately one step per 50 Å or less) introduces errors in the measured structure that are negligible in comparison to other sources of inaccuracy associated with the methodology.

ACKNOWLEDGMENTS

G. Teeter and J. L. Erskine acknowledge support by the R. A. Welch Foundation and by NSF/DMR Grant No. 9623494. F. Shi and M. A. Van Hove acknowledge support by the Director, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

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