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Truncation-induced multilayer relaxation of the Al(110) surface

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Results from a low-energy electron diffraction (LEED) analysis of the Al(110) surface are presented and discussed. The results indicate that a multilayer relaxation exists in the Al(110) surface region such that the spacing between layers 1 and 2 has a relative change Δd_{12} of -8.5% from the bulk value, while $\Delta d_{23}=+5.5\%$, $\Delta d_{34}=+2.2\%$, and $\Delta d_{45}=+1.6\%$. When these results are compared with those from an independent LEED analysis, excellent agreement is found between results for Δd_{12} and Δd_{23}. However, a disagreement is found to exist between the results of the two analyses for Δd_{34}. When this disagreement is considered in relationship to predictions of a recent theory for the multilayer relaxation of metallic surfaces, the importance of future work to resolve this Δd_{34} discrepancy is apparent.

I. INTRODUCTION

The termination of a metal crystal by a surface significantly alters the coordinations about the surface-region atoms from those about bulk atoms. These changes in coordination cause the surface-region conduction-electron distribution to be different from that of the bulk, and this difference can lead to further modifications of the surface's crystallography. For example, recent low-energy electron-diffraction (LEED) analyses[1–6] have clearly demonstrated the existence of multilayer relaxation[7] for some clean metallic surfaces. The plausibility of truncation-induced relaxations of metallic surfaces has also been indicated by several theoretical investigations.[8–12] However, at the time this Al(110) investigation was begun, serious quantitative discrepancies existed between values of interlayer spacings determined by LEED analysis and the values predicted by theoretical calculations where results existed for the same surface. A possible explanation for such discrepancies was that none of the theoretical work had allowed the surface-region charge density to adjust self-consistently to any multilayer relaxation. In this regard, theoretical calculations of relaxations at a simple metal surface, such as Al(110), should be much easier to perform than those for a transition-metal surface. There was, therefore, motivation to investigate, using modern LEED analysis, for the possibility of multilayer relaxation in the Al(110) surface. The values determined for the interlayer relaxations of the Al(110) would then serve to assess predictions by improved theoretical models of the forces causing relaxation at the surface.

Although the Al(110) surface was one of the first surfaces studied by LEED analysis,[13–20] none of this early work considered the possibility of multilayer relaxation. Also, these LEED analyses of Al(110) did not produce, by today's standards, a satisfactory agreement between calculated and experimental *I-V* spectra. However, these analyses did suggest that the distance between the first and second atomic layers d_{12} was contracted from the bulk value (1.43 Å) by 5–15%, depending on the particular study.[13–20] As will be discussed, this analysis of Al(110) indicates a value in the middle of this range (8.5%), and excellent agreement has been obtained between the calculated and experimental *I-V* spectra.

During the course of this Al(110) investigation, some pertinent new results have appeared in the literature. Nielsen *et al.*[21,22] have also performed a LEED analysis for Al(110) in which the possibility of multilayer relaxation was considered. This means that the results presented here can be compared with those of an independent investigation, and such comparison can serve to test the reproducibility of conclusions reached by modern LEED analyses. Although some differences do exist between the results of the two analyses and a specific discrepancy is highlighted below, the results obtained for the first two interlayer spacings are remarkably close. Also during the tenure of this Al(110) investigation, an improved theoretical treatment for multilayer relaxation was developed and applied to several surfaces.[23] These new theoretical predictions are in good agreement with the LEED results for the first two interlayer spacings of Al(110), which adds credibility to both types of research.

II. EXPERIMENTAL DETAILS

The experimental *I-V* spectra for the Al(110) surface were obtained using procedures similar to those used to obtain spectra for a LEED analysis of the Cu(100) surface.[1,24] Since that analysis produced excellent agreement between experimental and calculated spectra, it is assumed that such experimental procedures are adequate for reliable surface-structure determination. Briefly, an Al(110) surface was prepared by aligning, cutting, and polishing an Al single-crystal boule to expose the (110) plane. The crystal was electropolished using a perchloric-acid—acetic-anhydride electrolyte, and then it was installed quickly into the LEED scattering chamber. Since this procedure minimized the amount of surface oxide formed, an atomically clean surface could be obtained easily by sputtering with 500-eV Ar^+ ions and then annealing at ~580 °C (melting point is 660 °C). Owing to the inertness of Al to the residual gases present in a baked

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ultrahigh-vacuum chamber (base pressure $<2\times10^{-11}$ Torr), the sample remained clean for several days (as verified using a cylindrical mirror analyzer (CMA) as an Auger-electron spectrometer). However, surface order was a problem. After the above treatment was performed, the surface tended to form small ordered domains which were misoriented with respect to each other. As a consequence, broadened, and even split, LEED beams were observed. However, if the surface was annealed close to the melting temperature and then slowly cooled, some ordered domains could be grown sufficiently large to produce a sharp, well-focused LEED spot pattern. However, even this type of surface always had a significant fraction of its area composed of small, misoriented domains. Nevertheless, a clean Al(110) surface could be prepared with well-ordered domains of sufficient area that enabled reliable, and reproducible, *I-V* spectra to be obtained.

After the surface was properly prepared, an equivalent-beam-averaging (EBA) technique[25,26] was employed to obtain experimental *I-V* spectra for later comparison with calculated spectra. That is, with the incident beam aligned normal to the surface, the sets of *I-V* spectra for all symmetrically equivalent LEED beams were collected with a Faraday cup, compared to see that they were as similar as experimentally possible, and then data for symmetrically equivalent beams were averaged to produce a mean spectrum as a function of the energy of the incident electrons. This EBA technique, as has been previously demonstrated,[25,26] serves to reduce the effects of some possible systematic errors in LEED (e.g., those due to beam misalignment and divergence, and also due to some surface defects). Reducing the effects of such errors enables the surface's crystallography to be determined more precisely.[1] For Al(110), the EBA *I-V* spectra were obtained for each of the nine lowest-order, symmetrically inequivalent sets of beams. However, due to limitations caused by the physical restraints of the Faraday cup inside the vacuum chamber, data for the $\{10\}$ diffraction beams could only be obtained over a limited energy range. Because of the limited amount of data, the (10) *I-V* spectrum was not included in the analysis. However, it was consistent with the analysis of the other beams.

In this investigation the experimental spectra were collected with the sample maintained at room temperature, while the spectra obtained by Nielsen *et al.*[21,22] were for a sample temperature of 100 K. Considering the relatively simple electronic structure of Al, this temperature difference would not be expected to affect the Al(110) surface crystallography to within limits detectable by LEED. However, since the data of Nielsen *et al.* were collected for a lower temperature with corresponding reduction in atomic vibrations, some higher-energy peaks in their *I-V* spectra are more intense relative to lower-energy peaks. Other differences between the methods used to obtain the two sets of experimental spectra were that Nielsen *et al.* used a spot photometer over the energy range 40–350 eV, while this study analyzed data, which were measured using a Faraday cup, in the energy range 50–300 eV. In addition, the beams were indexed differently in the two studies. For example, the (10) beam in this study corresponds to the (01) beam in the report by Nielsen *et al.*

III. CALCULATIONAL DETAILS

Information concerning multilayer relaxation of the Al(110) surface was obained from the experimental EBA spectra by comparing them with results from dynamical LEED calculations. These were performed by first calculating layer-scattering matrices, as defined by Eq. (4.49) of Pendry,[27] and then using renormalized forward scattering (RFS) perturbation[28] to calculate the interlayer multiple scattering. All necessary computer codes were developed independently at Oak Ridge National Laboratory, and have been checked to insure their correctness by comparing results from them with numerous LEED calculational results which exist in the literature. Specific detailed tests were also made for Al(110) concerning numerical convergence of the calculational results. In these tests the total number of spatial lattice points included in the layer sums, the number of scattering phase shifts, and the number of beams used in RFS were all increased until adequate convergence was obtained. The RFS results also were compared selectively with results obtained using reverse-scattering perturbation[29] to guard against computational instabilities.

Since the computer codes were programmed with reasonable care, and normal-incidence calculations enable rotational and mirror symmetries to be exploited, the Al(110) calculations performed for this investigation required the expenditure of only relatively modest amounts of computer time. For example, fully converged calculations required only 0.30 sec of central-processing-unit (CPU) time on an IBM 3033 computer for an electron energy of 50 eV, and 1.54 sec of CPU time for an energy of 300 eV. These efficient computer codes enabled hundreds of sets of calculations to be performed for the Al(110) surface.

All the calculations performed during this investigation could be divided approximately into two categories. In one category the structural parameters (i.e., values for interlayer spacings) of the surface were fixed, and the customary nonstructural parameters were varied to determine the best values to use for Al(110). These nonstructural parameters were the scattering potential, the imaginary component of the optical potential, V_{oi}, to simulate electron-beam absorption, and a single Debye temperature Θ_D for the entire surface region to mimic the effects of atomic vibrations. In the second category of calculations the nonstructural parameters were held constant, while the values for the first few interlayer spacings were varied to determine their best values. In both categories of calculations, the optimal parameter values were determined by comparing calculated *I-V* spectra with the eight EBA experimental spectra. During such comparisons, the real component of the optical potential, V_{or}, was varied to obtain the best overall fit between the calculated and experimental spectra. After some self-consistent iteration between the two calculational categories, final optimized values were obtained for both structural and nonstructural parameters.

The experimental and calculated spectra were compared using reliability factors (*R* factors). In order to insure that use of a specific *R*-factor algorithm did not introduce any systematic distortion into our analysis, two very distinct single-beam R factors were employed. These were R_{ZJ} as defined by Zanazzi and Jona,[30] and R_2 defined by van Hove *et al.*[31] The factor R_{ZJ} was designed in an attempt to weigh those features that experienced investigators would use in a visual comparison of spectra, while R_2 is a measure of the mean-square difference between experimental and calculated spectra. The eight-beam R factors quoted herein are energy-weighted averages of the individual single-beam R's, and were calculated following the prescription given by Eqs. (14) and (16) of Zanazzi and Jona.[30]

IV. RESULTS

Nonstructural parameters were first optimized for the case where R_{ZJ} was used to compare spectra, and where only the first and second interlayer spacings were allowed to differ from the bulk value. The best values, resulting from self-consistent iteration between the two categories of calculations described in the preceding section, were $\Theta_D = 470$ K, $V_{oi} = 4.7$ eV for all energies, and phase shifts obtained from the Moruzzi-Janak-Williams band-structure potential.[32] Use of these values has led to a minimum, eight-beam R_{ZJ} value of 0.036 for relative changes, from the bulk value, of the first interlayer spacing, Δd_{12}, of -8.9%, and of the second, Δd_{23}, of $+5.9\%$. This minimum was obtained for $V_{or} = 10.4$ eV. The above set of nonstructural parameters were used to perform sets of calculations for 81 different pairs of $(\Delta d_{12}, \Delta d_{23})$ values. In these, Δd_{12} was varied from -14.0% to -4.0% and Δd_{23} was varied from $+2.0\%$ to $+12.0\%$, with Δd_{ij} incremented in steps of 1.25%. The results from these calculations have been used to construct Fig. 1. Each R_{ZJ} value of this figure is the minimum at the respective $(\Delta d_{12}, \Delta d_{23})$ point when V_{or} was varied. Although the point for the truncated bulk surface [i.e., the (0,0) point] is not plotted in Fig. 1, a simple visual extrapolation indicates that R_{ZJ} is reduced by about a factor of 2 from the case of no relaxation, the (0,0) point, to the case of best agreement, the $(-8.9\%, +5.9\%)$ point. This must be considered as strong evidence that multilayer relaxation exists in the Al(110) surface.

Since the electron penetration is attenuated, less information concerning interlayer spacings deeper into the crystal is available than for the spacings of layers which are close to the surface. It is this fact that causes the contours of constant R_{ZJ} of Fig. 1 to have their elliptic appearance. That is, the value of R_{ZJ} changes more with variation of Δd_{12} than with Δd_{23}. Regardless, we have performed calculations where Δd_{34} was varied. For these calculations the same nonstructural parameters were used, and the $(\Delta d_{12}, \Delta d_{23})$ pairs were fixed at the values producing the minimum R_{ZJ} of Fig. 1. Results are presented in Fig. 2 for the eight-beam R_{ZJ} value as a function of Δd_{34}. A smooth R_{ZJ} variation was obtained, and its value was reduced from 0.036 for $\Delta d_{34} = 0\%$ to the minimum value of 0.034 for $\Delta d_{34} = +2.2\%$. Each point of the curve of Fig. 2 is the respective minimum at the Δd_{34} value when V_{or} was varied, with $V_{or} = 9.8$ eV producing the overall minimum at $\Delta d_{34} = +2.2\%$. Also, consistency among the results for the individual LEED beams provides corroborating evidence for d_{34} being expanded from the bulk value. In these results, the value of the single-beam R_{ZJ} for seven of the eight analyzed beams decreased as Δd_{34} was changed from 0% to $+2.2\%$. Only the value of the R_{ZJ} for the (21) beam increased, specifically from 0.023 to 0.028.

Figure 3 contains plots of calculated and experimental I-V spectra. The calculated spectra of Fig. 3 are those which produced the minimum in the R_{ZJ} curve of Fig. 2. Associated with each calculated spectrum is the value for

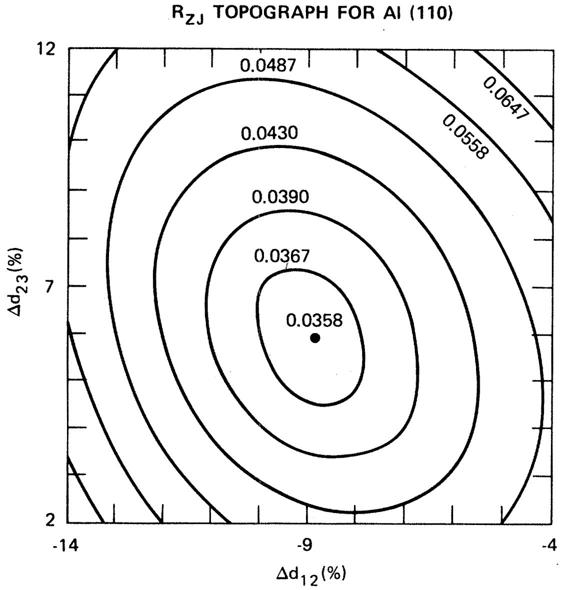

FIG. 1. Eight-beam R_{ZJ} topograph as a function of the relative changes of the first two interlayer spacings of Al(110). [The (10) beams are diffracted with azimuths in the planes determined by the surface normal and a surface ⟨100⟩ direction.]

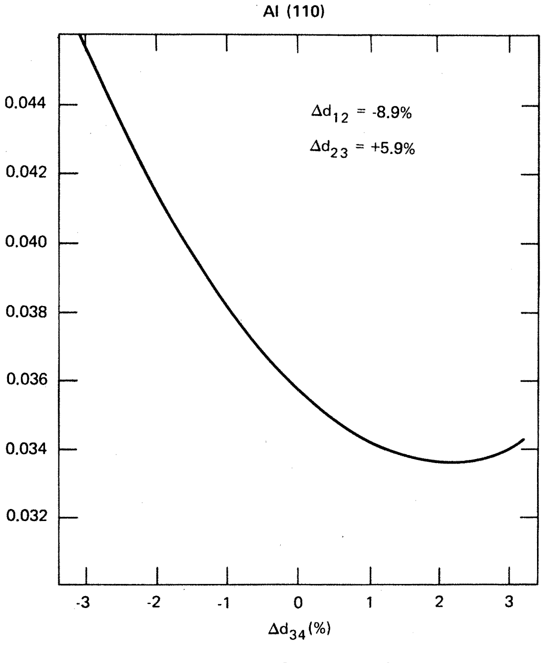

FIG. 2. Eight-beam R_{ZJ} as a function of the relative change of the spacing between the third and fourth atomic layers of the Al(110) surface.

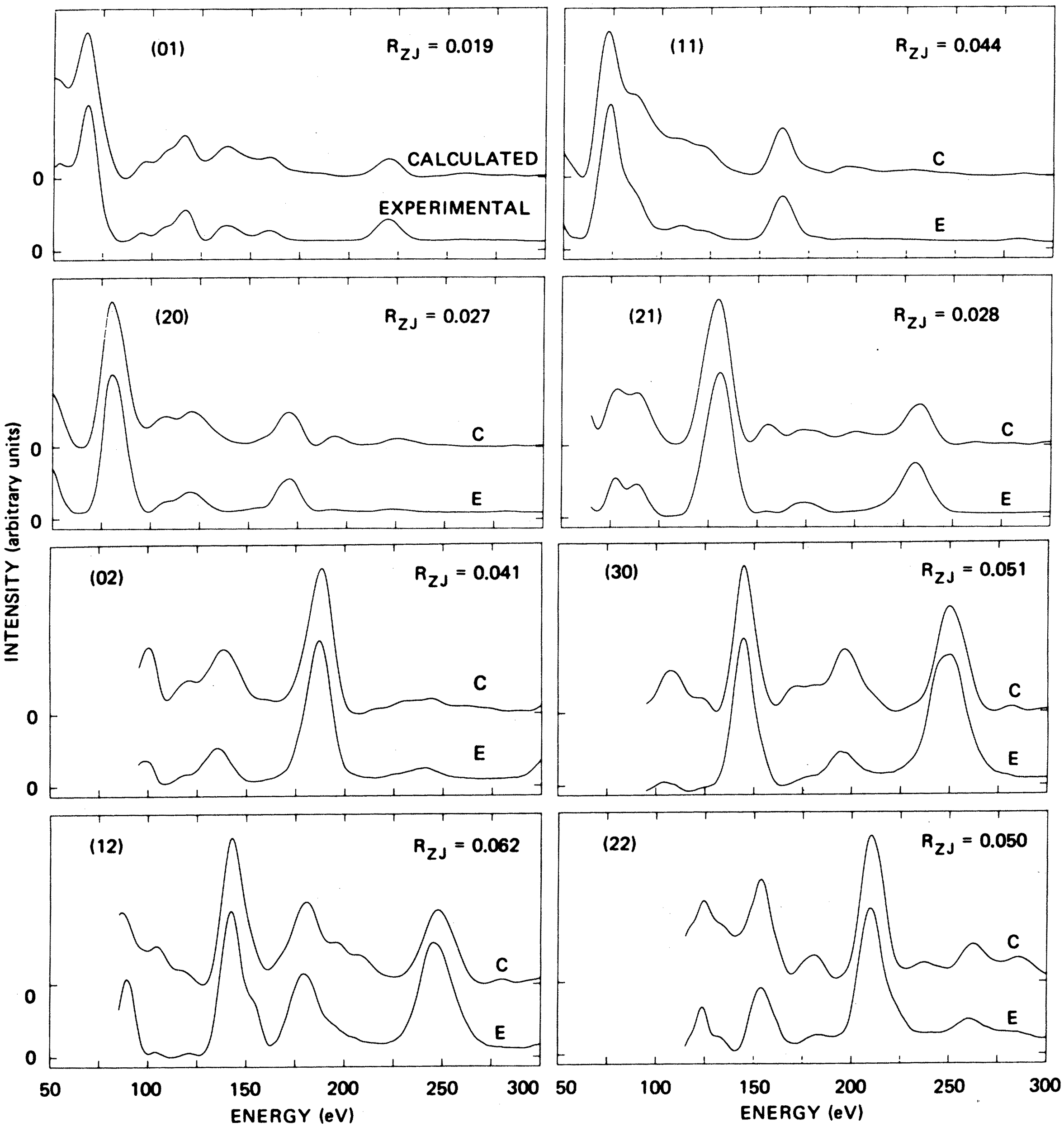

FIG. 3. Calculated (top curves) and experimental (bottom curves) *I-V* spectra for the Al(110) surface. The calculated spectra are for $\Delta d_{12} = -8.9\%$, $\Delta d_{23} = +5.9\%$, $\Delta d_{34} = +2.2\%$, and all other spectra are for $\Delta d_{ij} = 0\%$. The nonstructural parameters employed in the calculations are described in the text.

the single-beam R_{ZJ} which resulted when it was compared with the corresponding EBA experimental spectrum. These R_{ZJ} values are very small and indicate[30] that an excellent agreement between the calculated and experimental *I-V* spectra has been obtained.

Attempts were made also to determine whether any relaxation could be detected between layers 4 and 5, which is denoted as Δd_{45}. With the use of the same set of nonstructural parameters as before and fixing the first three Δd_{ij} at the values used to obtain the calculated spectra of Fig. 3, it was found that the eight-beam R_{ZJ} value was further reduced from 0.034 for $\Delta d_{45} = 0\%$ to 0.032 for $\Delta d_{45} = +1.6\%$. Also, the values of the single-beam R_{ZJ} for six of the eight analyzed beams decreased when Δd_{45} was changed from 0% to + 1.6%.

A detailed series of calculations also were performed where the R_2 factor[31] was employed to compare experimental and calculated *I-V* spectra. The procedures followed were similar to those used when R_{ZJ} was employed for the comparison. First, the best set of nonstructural parameters was determined to use with R_2. These parameters included $\Theta_D = 570$ K, $V_{oi} = 4.0$ eV for all energies, and phase shifts obtained from a band-structure potential tabulated by Snow.[33] The values were then used in calculations for various sets of $(\Delta d_{12}, \Delta d_{23})$, with all the other Δd_{ij}'s fixed at zero. This analysis produced an overall, eight-beam, R_2 minimum value of 0.045 at $\Delta d_{12} = -8.1\%$ and $\Delta d_{23} = +5.2\%$ for $V_{or} = 10.7$ eV.

Fixing $(\Delta d_{12}, \Delta d_{23})$ at these values, Δd_{34} was then varied. With this variation a minimum R_2 value of 0.039 was obtained for $\Delta d_{34} = +2.1\%$ with $V_{or} = 9.9$ eV. For comparison, an R_2 value of 0.059 was obtained for $\Delta d_{34} = -2.0\%$. As for the calculational set where R_{ZJ} was employed to perform the comparisons, agreement for seven of the eight analyzed beams improved as Δd_{34} was changed from 0% to +2.1%. Again, only the single-beam R_2 value for the (21) beam increased. Fixing the first three Δd_{ij}'s at the above values, Δd_{45} was then varied. The eight-beam R_2 minimum was lowered to 0.037 for $\Delta d_{45} = +1.5\%$ with $V_{or} = 9.6$ eV. Here, all eight analyzed beams had at least a slight reduction in their single-beam R_2's as Δd_{45} was changed from 0% to +1.5%.

In order to determine the best set of values for the nonstructural parameters to be used when either R_{ZJ} or R_2 was employed to perform comparisons, it was necessary to perform more calculations than just those which are explicitly described above. In these other calculations the value for Θ_D was varied, and V_{oi} was varied not only in its magnitude but also in its functional form with energy. In addition, besides the two referenced above, several additional atomic potentials were used to obtain the scattering phase shifts. Many sets of nonstructural parameters were investigated, and values for Δd_{12} and Δd_{23} were determined which produced the overall minimum R values for the respective sets. Although numerous sets of values for the parameters were investigated in this work, it should not be implied that the search was truly exhaustive. Among all the sets tested, the two sets quoted above produced the lowest overall minimum R values for, respectively, R_{ZJ} and R_2, when Δd_{12} and Δd_{23} were varied simultaneously. However, if another set of values for the nonstructural parameters were used, the R factors had their overall minima at slightly different $(\Delta d_{12}, \Delta d_{23})$ pairs than those quoted above. For example, use of $\Theta_D = 500$, $V_{oi} = 4.5$ eV, and phase shifts from the Snow potential[33] gave the overall minimum value of 0.049 (to be compared with 0.036 for the "best" set referred to above) for the eight-beam R_{ZJ} at $\Delta d_{12} = 9.2\%$ and $\Delta d_{23} = +6.3\%$. This identical set of nonstructural parameters had the overall minimum of $R_2 = 0.056$ (compared with 0.045 for the "best" set) for $\Delta d_{12} = -8.4\%$ and $\Delta d_{23} = +4.9\%$. Thus, although this set of nonstructural parameters leads to significantly larger minima for R_{ZJ} and R_2 (respectively, 37% and 24% larger), the values of Δd_{12} and Δd_{23} producing the minima are reasonably close to those obtained for the "best" sets of nonstructural parameters. Similar results have been obtained for all other sets of nonstructural parameters investigated. For any set of nonstructural parameters, the values of Δd_{12} and Δd_{23} which produced the overall R-factor minima deviated from the values obtained for the "best" sets by at most $\approx 1\%$ of the bulk spacing.

All the results obtained during this analysis are easily summarized. The totality of results indicate that the Al(110) surface has a multilayer relaxation of (in %)

$$\Delta d_{12} = -8.5 \pm 1.0, \quad \Delta d_{23} = +5.5 \pm 1.1 \; ,$$

$$\Delta d_{34} = +2.2 \pm 1.3, \quad \Delta d_{45} = +1.6 \pm 1.6$$

[stated in actual bond lengths, $d_{12} = (1.310 \pm 0.014)$, $d_{23} = (1.510 \pm 0.016)$, $d_{34} = (1.463 \pm 0.019)$, and $d_{45} = (1.455 \pm 0.022)$ Å]. The quantities which bracket these values for Δd_{ij} are not to be interpreted as statistical error limits. Instead, these quantities were selected to be reasonable "range limits," and they were assigned after consideration of several factors. These factors were the values of Δd_{ij} obtained with the two different R factors, employed to compare I-V spectra; the values of Δd_{ij} which produce minima in R values as the nonstructural parameter values were varied over physically reasonable limits; the sensitivity of the R values with minor change of Δd_{ij} about the values which produced the minima; and the fact that the available experimental signal is attenuated for information deeper into the surface region. The use of these range limits is preferred rather than statistical error limits, since systematic errors could be present in the LEED analysis associated with both the experimental measurements and the approximations used as the basis for calculational simulation of the I-V spectra.

V. DISCUSSION

The visual agreement obtained between calculated and experimental I-V spectra for Al(110) (see Fig. 3) is excellent. Furthermore, the comparison of the calculated and experimental spectra of Fig. 3 has resulted in an eight-beam R_{ZJ} value of 0.034, which, to our knowledge, is the smallest multibeam R_{ZJ} value reported to date. Although nonstructural parameter values were varied and three structural parameter values (i.e., the Δd_{ij}'s) were adjusted in the process of obtaining the calculated spectra of Fig. 3, the excellent agreement obtained with the experimental spectra should not be considered just as a result to be expected from any type of parametric curve fitting, since the number of parameters used in the calculations are considerably fewer than the number of prominent features in the eight experimental spectra. Thus it is believed that the Δd_{ij}'s obtained in this analysis must reflect some realistic crystallographic features of the Al(110) surface.

In their LEED analysis of Al(110) Nielsen *et al.*[21,22] also obtained excellent agreement between calculated and experimental I-V spectra. The final agreement they obtained is of the same quality as that illustrated by Fig. 3, but any digression here concerning which agreement is better would not serve a useful purpose. The final[22] results of Nielsen *et al.* indicate a multilayer relaxation for Al(110) of (in %)

$$\Delta d_{12} = -8.6 \pm 0.8, \quad \Delta d_{23} = +5.0 \pm 1.1 \; ,$$

$$\Delta d_{34} = -1.6 \pm 1.2, \quad \Delta d_{45} = +0.1 \pm 1.3 \; .$$

The quantities after the ±'s in these values for Δd_{ij} are statistical error limits, which were obtained by a very detailed statistical analysis.

Since 1% of $d_{ij} = 0.014$ Å, the very close agreement between our results and those of Nielsen *et al.* for Δd_{12} (−8.5% vs −8.6%) and Δd_{23} (+5.5% vs +5.0%) is really quite remarkable for LEED results obtained at different laboratories using quite different procedures and calculations in their respective analyses. This is especially true when one considers the difficulties all investigators have encountered when attempting to prepare a clean Al(110) surface with a corresponding, sharp LEED spot pattern.

However, there is a discrepancy in the value of Δd_{34} as determined by Nielsen *et al.* [(-1.6 ± 1.2) %] and the value found in this study [$(+2.2\pm1.3)$ %]. The results differ not only in sign, but no overlap exists within the states ranges. At present the explanation of the difference is not known. One possibility is that it is related to a temperature dependence of the relaxation since in this study the sample was at room temperature, and in the other study it was at 100 K. If there were a temperature effect, it should affect Δd_{12} and Δd_{23} as well. Therefore, the discrepancy is probably not due to the temperature difference. A second possibility could be that the accuracy of both analyses is not as good as quoted. Efforts are being made to define experiments which will assess the problem of determining the accuracy of the measured *I-V* spectra. There are, however, results which suggest that the data in this study is accurate enough to support the conclusion that Δd_{34} is expanded by $\approx 2.2\%$.

Considerable evidence was accumulated in our investigation to suggest that d_{34} is expanded by about 2% from the bulk value. For example, an expansion was indicated when using the best set of nonstructural parameters for either R_{ZJ} or R_2. The change in eight-beam R_{ZJ} with Δd_{34} is illustrated by Fig. 2, and R_{ZJ} decreases from 0.041 for $\Delta d_{34}=-2\%$ to 0.034 for $\Delta d_{34}=+2\%$. Also, seven of the eight analyzed beams had a reduction in their single-beam R_{ZJ} as Δd_{34} was changed from 0% to $+2\%$. Such consistency must be considered as good evidence for d_{34} being expanded. When the best set of nonstructural parameters for R_2 were used in our investigation, with $(\Delta d_{12},\Delta d_{23})$ fixed at $(-8.1\%,+5.2\%)$, the eight-beam R_2 was 0.059 for $\Delta d_{34}=-2\%$, 0.045 for $\Delta d_{34}=0\%$, and 0.039 for $\Delta d_{34}=+2\%$. Again, seven of the eight analyzed beams had a reduction in single-beam R_2 as Δd_{34} was changed from 0% to $+2\%$. Therefore all of the above results would clearly indicate that d_{34} is expanded by about 2%. However, it is not known whether as much consistent evidence is contained in the results of Nielsen *et al.* to indicate that d_{34} is contracted by about 2%, since they employed only R_2 to compare spectra and did not quote the same type of details concerning the change in single-beam R_2's with variation of Δd_{34}. Regardless, it appears that a genuine discrepancy exists concerning Δd_{34}. Also, it is important that this discrepancy be resolved, since, as is discussed below, the sign and magnitude of Δd_{34} can be useful in testing theoretical predictions of multilayer relaxation.

The theoretical literature concerning the multilayer relaxation of metallic surfaces has been summarized elsewhere;[1,2,12,22,23] thus only very pertinent details need to be included here. Also, an excellent tabulation of the various theoretical predictions for the first few Δd_{ij}'s of Al(110) has been given by Andersen *et al.*[22] in their Table IV. As an illustration of the difficulties associated with the development of a reliable theory for multilayer relaxation, it is noted that during the last few years theoretical predictions of, e.g., Δd_{12} for Al(110), have varied from -26% to $+2\%$. This range of values is to be compared to -8.5% obtained in this LEED analysis and -8.6% obtained by Andersen *et al.*[22] It is also important to note that none of the theoretical calculations for Al(110) have been fully self-consistent in their treatment of the electronic response to the multilayer relaxation.

The most complete theoretical treatment available today for Al(110) appears to be that of Barnett *et al.*,[23] who have investigated several models of varying degrees of complexity and realism. Results for each of their models predict an oscillatory behavior for the Δd_{ij}; i.e., Δd_{12} is negative, Δd_{23} is positive, Δd_{34} is negative, etc. Also, Barnett *et al.* provide physical reasons why such oscillatory behavior is plausible. However, the magnitudes predicted for the Δd_{ij} differ significantly from model to model and, thus, are shown to be sensitive to assumptions about the electronic density of the surface region. For the most realistic model, denoted DLHBS (dipole-layer Hartree band structure) by Barnett *et al.*, their predictions are $\Delta d_{12}=-10\%$, $\Delta d_{23}=+4\%$, $\Delta d_{34}=-3\%$, and $\Delta d_{45}=0\%$. So the discrepancy between our work and the results of the model calculations of Barnett *et al.* concerns only the value for Δd_{34}.

In summary, some noticeable features have emerged when our results of a LEED analysis for the Al(110) surface were compared with experimental and theoretical results obtained by others. First, excellent agreement has been found for the values of Δd_{12} and Δd_{23} obtained in our LEED analysis and one performed by Andersen *et al.*,[22] which demonstrates that a high degree of reproducibility can be achieved by LEED for metallic surfaces. Furthermore, the LEED results for Δd_{12} and Δ_{23} are in good agreement with recent theoretical results,[23] which helps to verify that the theoretical formalism has the proper thrust. However, a discrepancy has emerged concerning Δd_{34}, since our result for this quantity disagrees both with a previous LEED result[22] and a theoretical result[23] which are in reasonable agreement with each other. But, as discussed above, considerable evidence exists in the results of our LEED analysis that $\Delta d_{34}=(+2.2\pm1.3)$ %. Therefore it is important that this Δd_{34} discrepancy be resolved, since its resolution can be crucial in providing a benchmark test for theories of multilayer relaxation. Such a test is important for more than just the eventual understanding of the geometric and electronic structures of clean, perfect, semi-infinite, metallic surfaces, since the theory of Barnett *et al.* for multilayer relaxation follows from a much more general theoretical formalism[34] for single-ion and pair-interaction potentials. This more general formalism could be applied to, e.g., the analysis of the energetics of single and randomly distributed defects such as voids and grain boundaries. That is, the formalism could provide theoretical predictions concerning systems where direct experimental information is difficult, if not impossible, to obtain.

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