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Low-energy electron diffraction study of multilayer relaxation on a Pb{110} surface

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A low-energy electron diffraction (LEED) experiment was carried out on a Pb{110} surface at −140 °C. Intensity data were collected for ten nondegenerate beams at normal incidence and 15 nondegenerate beams at $\theta = 15°$, $\phi = 0°$. Quantitative intensity analyses of the two sets confirmed the substantial contraction of the first interlayer spacing that was found by other workers with room-temperature ion-shadowing and -blocking measurements. The results of the LEED analyses, averaged over the two experimental data sets, are the following: first-interlayer spacing compressed by 16.3%, second-interlayer spacing expanded by 3.4%, and third-interlayer spacing compressed by 4.0%. The modified point-ion model can be made to predict relaxation values in good agreement with experiment for the first and the third layer, but not for the second, if the restoring force to bulk positions that opposes surface relaxation is made much smaller than in other metals.

I. INTRODUCTION

The phenomenon of multilayer relaxation of solid surfaces is well established thanks to a number of experiments on several metals.[1,2] The phenomenon is a consequence of the formation of a surface, which is usually accompanied by rigid translations of atomic layers in the surface region. The translations can be perpendicular or parallel to the surface plane, but the translational symmetry of the lattice is maintained within each layer. Therefore, the geometry of the low-energy electron diffraction (LEED) pattern obtained from a relaxed surface is unchanged with respect to that of the pattern expected from a bulk-terminated, unrelaxed surface. In the language of surface crystallography,[3] we say that the LEED pattern is 1×1 both before and after relaxation. Thus, mere observation of a LEED pattern cannot reveal the phenomenon—instead, the relative positions of the atoms in the surface region must be determined with suitable surface- and structure-sensitive techniques, e.g., with LEED by means of quantitative intensity analysis, or with ion scattering by means of ion shadowing and blocking. By 1987, multilayer relaxation had been reported in the literature for about 40 surfaces of 17 different metals.[2]

The experimental results revealed three significant trends. (1) Surfaces with $ABAB\cdots$ stacking usually exhibit compression of the first-, expansion of the second-, and compression of the third-interlayer spacing, the magnitude of the relaxation decreasing progressively into the bulk. Surfaces with $ABCABC\cdots$ stacking may exhibit different sequences, e.g., compression, compression, expansion, and compression. (2) On the surfaces of several metals with the same bulk structure, the magnitudes of the perpendicular relaxations are almost the same (e.g., on {110} surfaces of Al, Ag, Cu, and Ni, the first interlayer spacing is contracted by about 8–9 %, the second is expanded by about 3–4 %, and the third is contracted by about 1–2 %). (3) High-index surfaces have larger relaxations than low-index surfaces and, in general, the magnitude of the first-interlayer relaxation increases with the roughness of the surface[2] (roughness is defined as the reciprocal of the surface packing density), reaching up to about 25% for a roughness of about 4 (e.g., on a bcc {210} surface).

The experimental results of multilayer relaxation studies have challenged fundamental surface theory to explain and predict the phenomenon quantitatively. So far, first-principles calculations have been successful in treating the problem of simple (low-index) surfaces,[4,5] but the multilayer relaxation of more open (high-index) surfaces, which require a large number of parameters, may be too difficult for such a fundamental approach. More empirical theories, particularly those based on electrostatic models, have proven more suitable to handle general surfaces, and, in fact, provide both theoretical understanding and a quantitative description of the relaxation process. Such theories are based on the point-ion model of Finnis and Heine,[6] who describe a metal crystal in terms of nets of positive point ions embedded in a uniform background of electronic charge. In this model, surface relaxation is due to the fact that the unsymmetrical environment prevailing in the surface region produces strong forces on the ions in this region and thereby causes the ions to move within the surrounding rigid electron distribution to positions at which the forces vanish. However, the point-ion model gives much larger relaxations than experiment, as was shown by Landman and co-workers.[6] These authors therefore proceeded to add interactions between the ions and assumptions about the response of the electron charge in order to get agreement between theoretical predictions and experimental results.[7]

Jiang, Marcus, and Jona[8] (JMJ) suggested another way to reduce the relaxation produced by the uniform-charge distribution in the point-ion model. They considered the relaxation of an ion net as a balance between two forces: one due to the interaction with other layers (always pulling the top layer inward), the other due to the interaction with the background charge in the same layer (always pulling the layer toward its bulk position). The latter force, which may be due to the double layer that arises when the ions are displaced from their bulk positions, is too weak in the uniform-charge model, but can be made stronger by heaping up the charge around the ions. The simplest, most convenient way to achieve this goal is to introduce into the expression for the electrostatic energy an empirical parameter α, which, when larger than unity, effectively strengthens the restoring force that tries to pull the ion nets back to their bulklike equilibrium positions. The resulting so-called modified point-ion or α model has been very successful in fitting experimental values of multilayer relaxation on several surfaces of Fe and Al,[8] and the remarkable fact about this success is that one and the same value of the empirical parameter α is sufficient to fit experiment, namely $\alpha = 1.9$. That the choice of $\alpha > 1$ is equivalent to a nonuniform-charge distribution was demonstrated by building such a nonuniform-charge model and calculating the purely electrostatic energy of the system without adding an empirical parameter. Minimization of this energy showed that the agreement with experiment found by the α model could be well reproduced for the perpendicular relaxations and even improved for the parallel relaxations. The latter feature results from the fact that the nonuniform-charge model strengthens the restoring forces to bulk positions for displacements in *any* direction, whereas the α model strengthens restoring forces only for displacements in the perpendicular direction.[9]

New experiments, however, seem to reveal material-dependent differences in the magnitude of the relaxation and perhaps fundamental limitations of the modified point-ion model. A recent study of the multilayer relaxation of a {110} surface of Pb, by the ion-shadowing and blocking technique,[10] found a substantial contraction of the first-interlayer spacing by 15.8% at room temperature—about twice as large as the relaxation measured on other fcc {110} surfaces. The modified point-ion model can be made to produce such a large first-layer relaxation, but only by means of a much smaller value of the parameter α, namely about 1.2. Such a value of α produces compression of the first-interlayer spacing by 15.85%, expansion of the second by 7.3%, compression of the third by 2.9%, and expansion of the fourth by 1.2%. The agreement with the ion-scattering experiment is excellent for the compressions of the first- (experimental value 15.8%) and the third- (3.0%) interlayer spacings, and fair for the expansion of the second (2.7%).

This novel behavior of Pb{110} suggests two immediate tests: one is an independent determination of the multilayer relaxation of Pb{110} by LEED, and the other is an experimental test of whether or not the value 1.2 for the α parameter describes correctly the multilayer relaxation of Pb surfaces. The present paper reports the results of the first test. The results of the second will be reported elsewhere.

The interest in a quantitative LEED study of Pb surfaces lies also in the fact that, with the possible exception of the reconstructed Au{110} surface,[11] LEED analysis has not produced the kind of fit to experiment for high-atomic-number metals that it has produced for low- and medium-atomic-number metals (Al, Fe, Ni, Cu). The present study of Pb{110}, described below, shows that while the set of parameters that produces the "best" fit to the LEED experiment is in good agreement with the ion-scattering results, the fit of calculated to experimental intensities is not as good as for other metals. A possible explanation for this fact will be discussed.

This paper is organized as follows. The experiment is described in Sec. II, the intensity calculations are explained in Sec. III, the results of the analysis are presented in Sec. IV, and the conclusions are discussed in Sec. V.

II. EXPERIMENT

A thin plate ($8 \times 4 \times 2$ mm^3) was cut from a larger Pb single-crystal ingot in such a way that the major surfaces were perpendicular to a $\langle 110 \rangle$ direction, as determined by Laue x-ray-diffraction patterns. The platelet was then lapped and polished with alumina-powder slurries with successively decreasing grain sizes (1, 0.3, and 0.05 μm), the plane of one of the major surfaces being kept on {110} to within ±0.5°. The final treatment, just prior to insertion into the experimental chamber, was a chemical polish consisting of 30-s agitation in a 2:1 mixture of acetic acid and hydrogen peroxide followed by a rinse in running water. The final surfaces appeared metallic and shiny, although not mirrorlike.

In the specimen holder, the sample was firmly clipped to a molybdenum platelet welded to a copper braid. The latter, in turn, was welded at the opposite end to a stainless-steel tube that could be filled with liquid nitrogen. The copper braid allowed limited rotation of the sample around an axis in the plane of the surface (θ rotation) and around an axis perpendicular to the surface (ϕ rotation). A hole in the molybdenum platelet allowed the back surface of the Pb sample to be exposed to electron bombardment.

In the experimental chamber (base pressure $< 10^{-10}$ Torr) the front surface of the Pb platelet was subjected to several cycles of Ar-ion bombardments (5×10^{-5} Torr, 375 V, 10 μA) of 1 h each, followed by $\frac{1}{2}$-h anneals at 240 °C. After ten cycles, Auger-electron-spectroscopy (AES) spectra showed no impurity signals, above the noise level, from S, O, or C.

Low-energy electron diffraction (LEED) on the clean, room-temperature, Pb{110} surface produced 1×1 patterns with high background, which increased with increasing energy of the incident electrons. On the fluorescent screen of a display-type LEED apparatus, the diffraction spots were discernible above background only below 110 eV (the Debye temperature of Pb is quoted in the literature as 105–108° K).

The Pb sample was cooled by filling the attached stainless-steel tube (see above) with liquid nitrogen. Thermal equilibrium was reached after 40 min, the sample temperature being then −140 °C, as determined with a thermocouple attached to a dummy sample in a calibration run. At −140 °C the LEED pattern was a sharp, low-background 1×1 pattern that was visible on the fluorescent screen up to electron energies of 250 eV.

LEED intensity spectra (*I-V* curves) were measured with a microcomputer–television-camera system described elsewhere[12] for incident-electron energies varying between 20 and 200 eV. Two sets of intensity data were collected, one for normal incidence ($\theta=0°$) and the other for $\theta=15°$, $\phi=0°$. In both sets, several degenerate spectra were measured and then averaged for use in the intensity analysis. The azimuthal orientation of the sample is depicted schematically in Fig. 1 in relation to the electron-gun location. The direction of the x axis on the Pb{110} surface was chosen along $\langle 01\bar{1}\rangle$. The LEED spectra collected were the following: for $\theta=0°$, 10, 01, 11, 20, 02, 21, 12, 22, 03, 13 (ten nondegenerate spectra, averaged from a total of 20 degenerate spectra); for $\theta=15°$ and $\phi=0°$, 00, 10, 01, 11, $\bar{1}\bar{1}$, 02, $\bar{2}0$, $\bar{1}\bar{2}$, $\bar{2}\bar{1}$, $\bar{2}\bar{2}$, $\bar{3}0$, $\bar{3}1$, $\bar{1}\bar{3}$, $\bar{2}\bar{3}$, $\bar{3}\bar{2}$ (15 nondegenerate spectra, averaged from a total of 19 degenerate spectra).

In view of the forthcoming discussion of the structural results (Sec. V), it may be appropriate to give a few details about the procedure adopted for collection of the intensity data. First, the surface was subjected to one cycle of Ar-ion bombardment and anneal as described above, and an AES spectrum was taken to check the cleanness of the surface. Second, the sample was cooled to about −140 °C, several degenerate LEED spectra were recorded, and the sample orientation adjusted to get normal incidence of the primary electron beam. Third, after achieving normal incidence, intensity data were collected, usually for about six to eight beams at one time, with the primary energy varying between 20 and 200 eV, and several scans were made to improve the signal-to-noise ratio. Finally, the sample was allowed to warm up to room temperature and another AES spectrum was recorded. The whole procedure required usually 2–3 h, but the final AES spectrum revealed no visible increase of impurity levels. Each of the two data sets ($\theta=0°$ and 15°, $\phi=0°$) were collected three times *ex novo,* and corresponding LEED spectra were judged to be identical to one another by visual inspection.

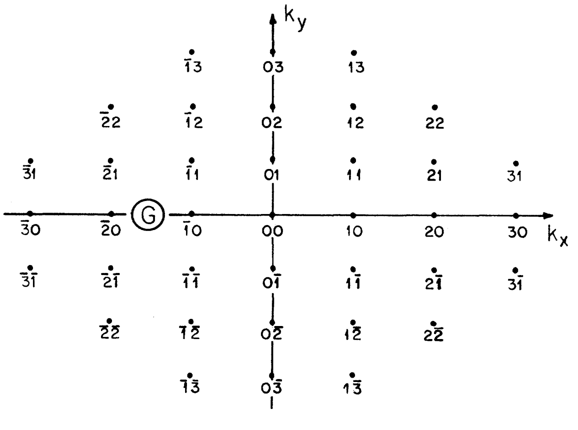

FIG. 1. Schematic LEED pattern from Pb{110} with the beam indices used in the present work. The circled *G* marks the position of the electron gun during collection of non-normal-incidence intensity data.

For the purposes of structure analysis, the LEED spectra were normalized to constant incident current and reduced to minimum background.

III. INTENSITY CALCULATIONS

For all structural models tested, the LEED intensities were calculated with Jepsen's CHANGE computer program,[13] with ten phase shifts and 73 beams (for energies up to 200 eV). Several Pb potentials were tested in the course of the analysis. At first, relativistic phase shifts were used as direct inputs into the CHANGE program, but they were found to produce numerical instabilities below about 100 eV and poor convergence above. Since CHANGE normally requires the input of a potential, and calculates the phase shifts internally at each energy as needed, three Pb potentials were calculated by superposition of appropriate charge densities. The charge densities that were used were relativistic, nonrelativistic (obtained from N. Christensen), and Herman-Skillman[14] charge densities. The corresponding potentials were labeled *R* (relativistic), NR (nonrelativistic), and HS (Herman-Skillman), respectively. The LEED spectra calculated with any of the potentials[15] were visually indistinguishable from one another, a fact which made the choice of potential to be used in the analysis immaterial. The *R* potential alone was used for the refinement, but the final model was tested with the NR and the HS potentials as well.

The inner potential was chosen initially to be $V_0=-(10+4i)$ eV, but the real part was varied as a fitting parameter during the analysis. The final value of the inner potential was $V_0=-(6+4i)$ eV with an experimental error of ±2 eV in the real part. The amplitude of the atomic vibrations (related to the Debye-Waller factor) was also varied during the analysis in order to improve the fit between theory and experiment, the final value being $\langle u^2\rangle^{1/2}=0.14$ Å.

IV. ANALYSIS

Evaluation of the correspondence between calculated and experimental LEED spectra was done qualitatively by visual comparison and quantitatively by means of the Zanazzi-Jona reliability factor r_{ZJ}.[16] The bulk lattice constant of Pb was taken as $a_0=4.9502$ Å at 25 °C and extrapolated to −140 °C by means of the experimental expansion coefficient for Pb published in the literature[17] to become $a_0=4.9265$ Å.

The structural parameters that were varied in the course of the analysis were the first three interlayer spacings: d_{12} (with change denoted Δd_{12}), d_{23} (with change Δd_{23}), and d_{34} (with change Δd_{34}). The initial variations spanned large ranges (−0.33 to +0.15 Å), but the refinement was done between −0.26 and −0.30 Å in steps of 0.02 Å for Δd_{12}, between −0.2 and +0.2 Å in steps of 0.05 Å for Δd_{23}, and between -0.12 and $+0.12$ Å in steps of 0.03 Å for Δd_{34}.

For the data at normal incidence the parameter set that produced the lowest r_{ZJ} factor (called model *M*0) was

$$\Delta d_{12} = -0.28 \pm 0.03\ \text{Å}\ ,$$

$$\Delta d_{23} = 0 \pm 0.03\ \text{Å}\ ,$$

$$\Delta d_{34} = -0.085 \pm 0.03\ \text{Å}\ ,$$

with $r_{ZJ} = 0.27$ for the *R* potential, 0.28 for the NR potential, and 0.27 for the HS potential. The quality of the fit can be judged from Fig. 2.

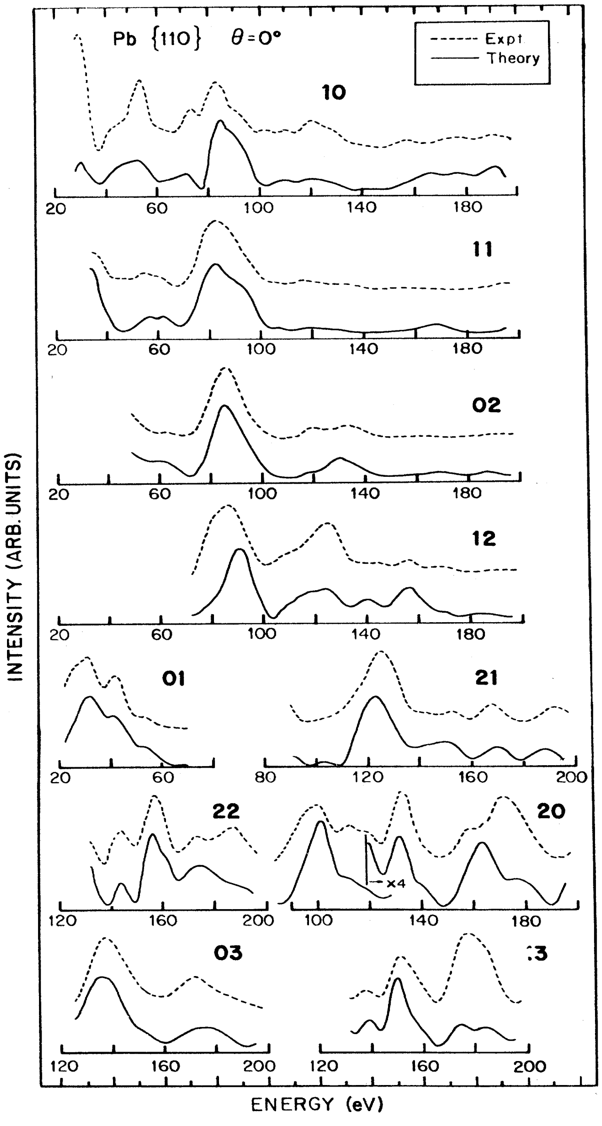

FIG. 2. LEED intensity spectra from Pb{110} at normal incidence. Dotted curves, experiment; solid curves, theory for the *M*0 model discussed in the text.

The *M*0 model, however, did not produce the best possible fit to the data at $\theta = 15°$, $\phi = 0°$ (the r_{ZJ} factor rose to 0.40). Independent refinement of the structure using only the non-normal-incidence data (the refinement included optimization of the angle of incidence θ) produced a different set of structural parameters (called the *M*15 model), viz.,

$$\Delta d_{12} = -0.29 \pm 0.03\ \text{Å}\ ,$$

$$\Delta d_{23} = +0.11 \pm 0.03\ \text{Å}\ ,$$

$$\Delta d_{34} = -0.06 \pm 0.03\ \text{Å}\ ,$$

with r_{ZJ} factors 0.34, 0.31, and 0.34 for the *R*, NR, and HS potentials, respectively. The quality of the fit to experiment can be judged in Figs. 3 and 4.

The difference between *M*15 and *M*0 is obviously within the estimated experimental error for Δd_{12} and Δd_{34}, but largely outside for Δd_{23}. Model *M*15 produces a worse fit than *M*0 when tested against the normal-incidence data ($r_{ZJ} = 0.28$ and 0.30 for the *R* and NR potentials, respectively). Lacking a satisfactory explanation

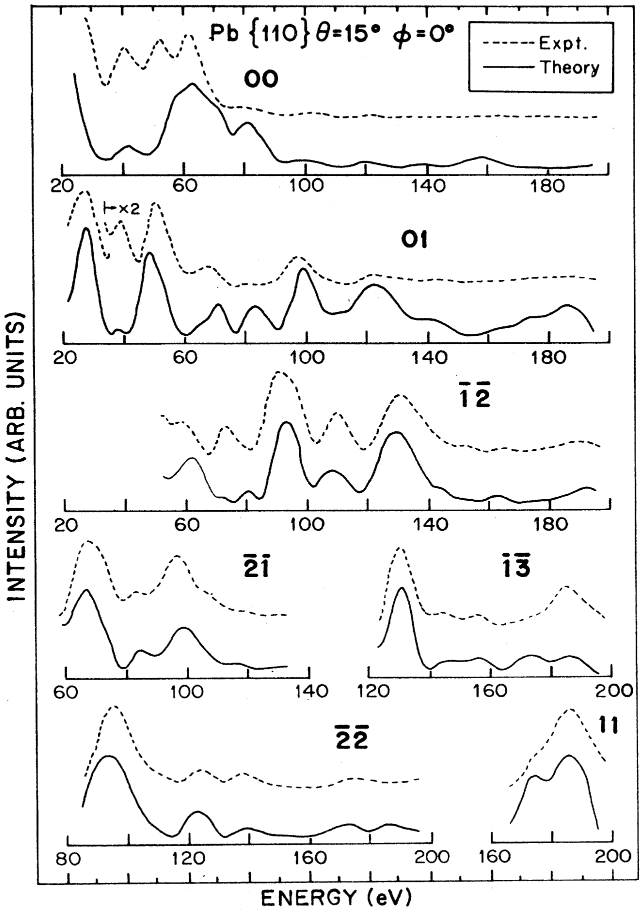

FIG. 3. LEED intensity spectra from Pb{110} for $\theta = 15°$, $\phi = 0°$. Dotted curves, experiment; solid curves, theory for the *M*15 model discussed in the text.

for this discrepancy (see Sec. V), we quote the final results as the average between *M*0 and *M*15 as follows:

$$\Delta d_{12} = -0.285 \pm 0.03\ \text{Å}\quad (16.3\%\ \text{compression})\ ,$$

$$\Delta d_{23} = +0.06 \pm 0.1\ \text{Å}\quad (3.4\%\ \text{expansion})\ ,$$

$$\Delta d_{34} = -0.076 \pm 0.03\ \text{Å}\quad (4.0\%\ \text{compression})\ ,$$

with the bulk interlayer spacing $d_{\text{bulk}} = 1.74$ Å at $-140\,^\circ\text{C}$.

V. DISCUSSION

Overall, the agreement between calculated and experimental LEED spectra is at best fair, certainly not as good as for the surfaces of other metals. The r_{ZJ} factors reflect this judgement adequately. In judging the reliability of the structure, it should be remembered that the present analysis is based on a notably larger data base than is normally available (25 nondegenerate LEED spectra for a total-energy range of 2689 eV). Nevertheless, the fit of some spectra, e.g., that of the 00 beam at $\theta = 15°$, $\phi = 0°$, is not very satisfactory (see Fig. 3).

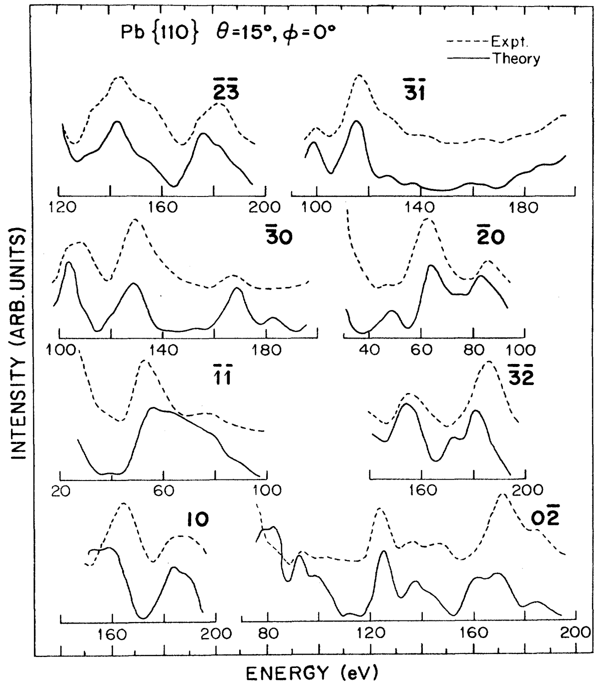

FIG. 4. LEED intensity spectra from Pb{110} for $\theta = 15°$, $\phi = 0°$. Dotted curves, experiment; solid curves, theory for the *M*15 model discussed in the text.

This overall mediocre fit to experiment, added to the fact that the *M*0 model, which fits the normal-incidence data best, does not give the best fit to the off-normal-incidence data well, and *vice versa* for the *M*15 model, requires an explanation. One might initially suspect the experimental data. However, critical examination of how the data were collected, and the number of repetitions, leads to the conclusion that the experimental reproducibility was excellent. The 00 spectrum at $\theta = 15°$, $\phi = 0°$, for example, was carefully measured several times and never diverged from the experimental curve depicted in Fig. 3. Thus, although unknown errors can never be excluded, the experimental data obtained here are, in our opinion, rather reliable. A second source of suspicion is the analysis itself. Can the structural parameters be optimized further, so that a model can be found which fits both sets of experimental data equally well, and better than *M*0 and *M*15? The answer is: unlikely. As far as the first three interlayer spacings are concerned, parameter space has been covered rather thoroughly, at least within a reasonable range of values. The probability that variations of the fourth- and the fifth-interlayer spacings, d_{45} and d_{56}, would make a large difference is rather small (the modified point-ion model, with $\alpha = 1.2$, predicts $\Delta d_{45} = +1.22\%$ and $\Delta d_{56} = -0.48\%$).

A third, more probable, cause of the mediocre fit to experiment is the Pb potential. This suspicion is reasonable because, despite the mediocre fit to experiment, the results of the LEED analysis are in good agreement with those of the ion-scattering experiment, as summarized in Table I. There is reason to believe, therefore, that the

TABLE I. Multilayer relaxation of Pb{110}. Δd_{12} denotes the change in first-interlayer spacing, Δd_{23} the change in second-interlayer spacing, and Δd_{34} the change in third-interlayer spacing; $\Delta^* = \Delta d_{23} + 0.75\,\Delta d_{34}$ (relation defined in Ref. 10). All data in %. ($d_{\text{bulk}} = 1.74$ Å.)

Source	Δd_{12}	Δd_{23}	Δd_{34}	Δ^*
Ion scattering: RT expt.[a]	-15.8 ± 2.5	$+2.7$	-3.0	$+0.5 \pm 2.5$
Ion scattering: 29-K expt.[b]	-17.2 ± 0.5	$+8.0 \pm 2.0$		
LEED: 130-K expt.[c]	-16.3 ± 1.7	$+3.4 \pm 5.7$	-4.0 ± 1.7	$+0.4 \pm 7.0$
Theory: energy minimum[a]	-15.9	$+7.9$	-6.8	$+2.8$
Theory: α model ($\alpha = 1.2$)	-15.9	$+7.3$	-2.9	$+5.1$
Theory: α model ($\alpha = 1.185$)	-16.28	$+7.65$	-3.07	$+5.3$

[a] Reference 10: LEED spectra calculated with the parameters from the ion-scattering experiment at room temperature (RT) produce a fit to the normal-incidence experiment with $r_{ZJ} = 0.33$.

[b] Reference 18.

[c] The relaxations quoted here are averages of the best models found with the normal-incidence and the $\theta = 15°$, $\phi = 0°$ data, respectively, viz., $\Delta d_{12} = -16.0\%$, $\Delta d_{23} = 0$, $\Delta d_{34} = -4.9\%$, ($r_{ZJ} = 0.27$ at $\theta = 0°$); and $\Delta d_{12} = -16.7\%$, $\Delta d_{23} = +6.3\%$, $\Delta d_{34} = -3.4\%$ ($r_{ZJ} = 0.34$ at $\theta = 15°$, $\phi = 0°$).

structure of clean Pb{110}, as described by the experimental results listed in Table I, is probably correct. In addition, although the potentials used in the LEED analysis had different origins, they led to essentially identical structures. We conclude that the structure is reliable, but a better potential might give a precise description of the LEED experiment, especially in the energy range below and around 100 eV. Conceivably, the potential itself could be adjusted to give a best fit to the experiment.

Our results confirm the statement of the ion-scattering experiment that the relaxation of Pb{110} is about twice as large as that of the low-atomic-number metals investigated so far. Table I shows that theory (either the energy-minimization scheme of Landman and coworkers[10] or the modified point-ion model[8]) fits the first-layer relaxation very well, but not the second-layer relaxation. The modified point-ion model requires $\alpha \cong 1.2$ to match the first-layer relaxation, and does well for the third-layer relaxation too, but is wrong by about a factor of 2 in the second-layer relaxation. The fact that the α parameter is 37% smaller for Pb than for Al, Fe, Ni, or Cu (for which $\alpha = 1.9$ provides a good description of the experimental results[8]) indicates that in Pb the restoring force that resists the relaxation is substantially weaker than in the other metals mentioned. A microscopic explanation of this fact is not available at this time, but may be related to the much smaller cohesive energy of Pb as compared to that of the 3*d* transition metals and even of Al.

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[1] D. L. Adams, L. E. Petersen, and C. S. Sorensen, J. Phys. C **18**, 1753 (1985).

[2] F. Jona and P. M. Marcus, in *The Structure of Surfaces II,* edited by J. F. Van der Veen and M. A. Van Hove (Springer, Berlin, 1987), p. 90.

[3] E. A. Wood, J. Appl. Phys. **35**, 1306 (1964).

[4] K. M. Ho and K. P. Bohnen, Phys. Rev. B **32**, 3446 (1985).

[5] C. L. Fu, S. Onishi, H. F. Jansen, and A. J. Freeman, Phys. Rev. B **31**, 1168 (1985).

[6] M. W. Finnis and V. Heine, J. Phys. F **4**, L37 (1974).

[7] U. Landman, R. N. Hill, and M. Mostoller, Phys. Rev. B **21**, 448 (1980); R. N. Barnett, U. Landman, and C. L. Cleveland, *ibid.* **27**, 6534 (1983); **28**, 1685 (1983); Phys. Rev. Lett. **51**, 1359 (1983).

[8] P. Jiang, P. M. Marcus, and F. Jona, Solid State Commun. **59**, 275 (1986).

[9] P. M. Marcus, P. Jiang, and F. Jona, Ref. 2, p. 100; in *Atomic Scale Calculations in Materials Science,* Mater. Res. Soc. Symp. Proc. No. 141, edited by J. Tersoff, D. Vanderbilt, and V. Vitek (MRS, Pittsburgh, 1989), p. 457.

[10] J. W. M. Frenken, J. F. Van der Veen, R. N. Barnett, U. Landman, and C. L. Cleveland, Surf. Sci. **172**, 319 (1986).

[11] W. Moritz and D. Wolf, Surf. Sci. **163**, L655 (1985).

[12] F. Jona, J. A. Strozier, Jr., and P. M. Marcus, in *The Structure of Surfaces,* edited by M. A. Van Hove and S. Y. Tong (Springer, Berlin, 1985), p. 92.

[13] D. W. Jepsen, Phys. Rev. B **22**, 814 (1980); **22**, 5701 (1980).

[14] F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, NJ, 1963).

[15] The CHANGE program calculates the phase shifts from the potential by means of the nonrelativistic Schrödinger equation.

[16] E. Zanazzi and F. Jona, Surf. Sci. **62**, 61 (1977).

[17] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys* (Pergamon, New York, 1958).

[18] J. W. M. Frenken, F. Huussen, and J. F. Van der Veen, Phys. Rev. Lett. **58**, 401 (1987).