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# Low-Energy-Electron-Diffraction Intensities from Ag{001}. II. Theory

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The angular dependence of low-energy-electron-diffraction spectra from Ag{001} is reexamined. The energy dependence of the imaginary part of the scattering potential is determined by comparing the measured total elastic current reflected by the surface with that calculated for a rigid lattice, thereby substantially removing the dependence on lattice motion and surface roughness. This energy-dependent complex potential is then used to calculate several specular and nonspecular spectra for incident angles up to 50°. Except for the spectra at 50° incidence, all calculated spectra are in very good agreement with the observed spectra as far as peak positions and shapes are concerned. As expected, the observed intensities are always somewhat less than calculated intensities because of the imperfections of the surface used in the experiment.

## I. INTRODUCTION

In earlier papers[1-3] we have examined in detail the low-energy-electron-diffraction (LEED) intensities obtained from surfaces of aluminum, copper, and silver in regard to dependence upon energy and the angle of incidence of the primary electron beam as well as upon the model assumed for the termination of the bulk structure at the surface. The calculations were done with the layer-KKR (Korringa-Kohn-Rostoker) procedure, which applies the KKR method of band theory to a single atomic layer to give the scattering properties of that layer and then solves the multiple-scattering problem between layers with a systematic matrix procedure.[4] The crystal potential is supplemented by an imaginary part, called $\beta$, to take into account the short mean free path of electrons for inelastic electron scattering in the metals considered and in the energy range of interest to LEED, and by an inner potential $\Delta$ which gives the difference in energy between vacuum and the average potential between atoms (the muffin-tin zero). Correction for lattice motion is introduced by putting the average coherent and incoherent scattering of an atom (averaged over a Debye spectrum of lattice motion at each site) into the usual rigid-lattice formalism, as justified by Duke and Laramore.[5,6]

The agreement between calculated and observed LEED spectra was found to be good to excellent for two surfaces of aluminum[1-3] (viz., Al{001} and Al{111}) and two surfaces of copper[2,7] (viz., Cu{001} and Cu{111}), but was much less satisfactory for the Ag{001} surface.[1] Agreement for Al{110} was also good, but with certain clear discrepancies which we believe can be explained by the quality of the surface available for experimental measurement. A few other authors have also compared theory to experiment for aluminum and copper surfaces[8-13] and found mostly satisfactory agreement. We have not found other calculations to check against for Ag{001}, but the new experimental results[14] agree well with our calculation. This paper gives the theoretical treatment of the experiments described in the previous paper,[14] where we note that many of the features observed in the experimental Ag{001} spectra reported earlier[1] could not be reproduced with a bulk sample of silver. Thus, there is some evidence that the difficulties in the earlier experiments might be responsible for the unsatisfactory agreement between observed and calculated spectra found earlier. One object of this paper is to establish that the method of calculation is adequate for surfaces of silver by obtaining satisfactory agreement between theory and experiment.

In earlier work on Ag{111} we used a crystal potential in muffin-tin form from work on the band structure of silver, the self-consistent Hartree-Fock-Slater crystal potential calculated by Snow[15] with exchange-correlation parameter $\alpha = \frac{5}{6}$. This potential has been shown to be reasonably successful in reproducing Fermi-surface data for silver,[16] but was only partially successful[17] in reproducing Lagally's data[18] for Ag{111}, e.g., the calculated intensities were much larger than observed (about 7 times around 60 eV and 14 times around 100 eV). This discrepancy in intensities is common to all our calculations of the few LEED spectra for which absolute experimental data are available,[1,7] when the calculations are made with a constant value of the imaginary part $\beta$ of the crystal potential. The constant value used was chosen to approximate the imaginary part of the self-energy calculated for a uniform electron gas by Lundqvist,[19] assuming that one $s$ electron per silver atom enters the metallic electron gas of the crystal, and ignoring the con-

tribution of the $d$ electrons to the electron gas. In the present paper we develop a procedure to use experimental data to determine $\beta$ and its dependence upon energy, and then use the resulting function of energy $\beta(E)$ to calculate LEED spectra from Ag{001} at different incident angles. The calculation also requires a value for the inner potential $\Delta$; in all the calculations in this paper $\Delta$ has the magnitude 8 eV.

## II. ENERGY DEPENDENCE OF IMAGINARY PART OF THE CRYSTAL POTENTIAL

### A. Total Elastic Current

When comparing absolute intensities in observed and calculated LEED spectra of a given surface, it is necessary to consider many factors which tend to reduce the intensity of a given diffracted beam in the experiment. These factors are of three types: the inelastic scattering processes with other electrons in the interior of the solid, the diffuse scattering caused by the lattice motion, and the diffuse scattering caused by roughness and irregularities of the actual surface used in the experiment. In the theory, the inelastic scattering in the bulk is described by the imaginary part $\beta$ of the crystal potential and the lattice motion effects are taken into account by modifying the effective scattering phase shifts of the atoms as described elsewhere.[1,2,4-6] However, the theory assumes a perfect surface of a low-index plane, i.e., it does not consider diffuse scattering caused by surface irregularities and steps. Furthermore, it is difficult or impossible to distinguish between bulk inelastic scattering and phonon effects by comparing theory and experiment for various beams. These considerations suggest that since scattering due to surface irregularities is omitted, the calculated intensities are expected to be always larger than observed (an expectation that is confirmed in all cases examined), and we cannot fix $\beta$ by comparison between calculated and observed LEED spectra of individual beams.

A procedure to find $\beta$ that avoids the difficulties with surface irregularities noted above uses the *total* elastic scattering from the crystal, rather than the individual beam intensities. The total elastic scattering consists of the sum of the intensities in all beams plus the diffuse background (the electrons scattered out of the beams by both phonons and surface irregularities). We compare this total intensity with the calculated total intensity in all beams for a rigid lattice. Here, with a perfect surface, the electrons which would be scattered by phonons or surface roughness remain included in the beams. Hence this total scattering is comparable with the experimental total. With a given atomic potential the absolute intensity in the theoretical total scattering now depends only on one parameter, the inelastic scattering potential $\beta$. The theoretical total scattering can then be made to give the experimental result by adjusting $\beta$ at each energy, hence experiment can be used to determine $\beta(E)$.

A possible source of error in this procedure is that some of the electrons interacting with phonons and surface irregularities may be deflected so as not to emerge from the sample. Since we find, in general, that the reflected intensities in the beams are reduced by increase of $\beta$, we expect that this procedure will give an upper bound to $\beta$ since the total elastic current is underestimated by the measurement, which picks up only the electrons (back) scattered into the vacuum hemisphere. It is convenient to refer to this underestimate of the diffuse background as electron retention or, simply, retention. Certainly partial retention occurs for beams that are almost parallel to the surface. But since single-phonon scattering is known to peak around the elastic beam, and multiphonon scattering, although less strongly directed, is still greatest in the halos around the elastic beams, we believe the retention effect is small. The assumption of small retention for roughness effects agrees with the analysis of Laramore, Houston, and Park,[19] who estimate the effects of a distribution of surface steps on LEED beam intensities and profiles. Under certain assumptions they show, in fact, that the total integrated elastic intensity is independent of the distribution of steps in both size and thickness.

### B. Estimation of $\beta$

We begin by comparing, in Fig. 1, the total elastic current measured experimentally on an Ag{001} surface for an incident angle $\theta = 0°$ and that calculated with the layer-KKR method for a rigid lattice with a constant value of $\beta = 0.25$ Ry as derived from Lundqvist's jellium calculations.[20] The experimental curve was determined (in a conventional display-type LEED equipment) by biasing the sample negatively with respect to the grid-screen assembly, so as to collect *all* the elastic backscattered electrons, and measuring the electron current flowing through the fluorescent screen, which acts in this case as a collector. In the conventional geometry of a common LEED equipment, such a measurement would miss the electrons that are reflected specularly or close to specularly, as the 00 beam would return into the collimating tube and hence not be collected by the fluorescent screen. For this reason, the theoretical curve that should be compared with this experiment is one calculated with the exclusion of the 00 beam (middle curve in Fig. 1). It appears, in fact, that this curve bears more resemblance to the experimental curve than does the theoretical curve cal-

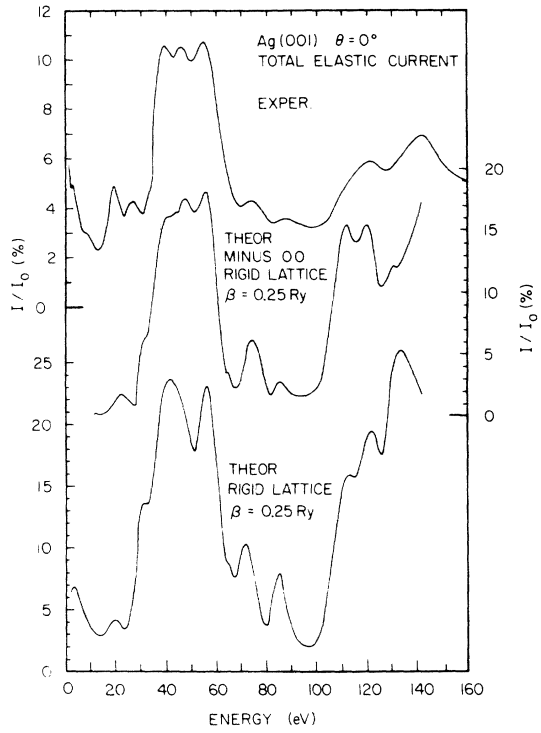


FIG. 1. Total elastic current reflected from Ag{001} at $\theta = 0°$. Top curve: experimental. Middle curve: calculated with constant $\beta = 0.25$ Ry for a rigid lattice with exclusion of the specular beam. Bottom curve: calculated with constant $\beta = 0.25$ Ry for a rigid lattice but including the specular beam. All calculated curves used a value of 8 eV for $\Delta$, the difference between the vacuum level and muffin-tin zero.

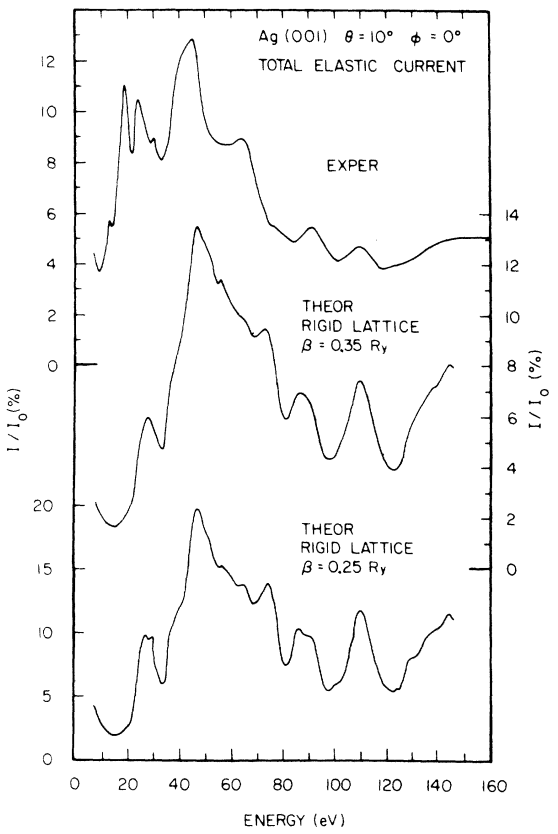


FIG. 2. Total elastic current reflected from Ag{001} at $\theta = 10°$, $\phi = 0°$. Top curve: experimental. Middle curve: calculated (rigid lattice, $\beta = 0.35$ Ry). Bottom curve: calculated (rigid lattice, $\beta = 0.25$ Ry).

culated with inclusion of the 00 beam (lower curve in Fig. 1). The quantitative agreement between theory and experiment is poor; we ascribe this to the value of $\beta$ chosen for the calculations.

Subtraction of the specularly reflected intensity is not needed if the angle of incidence is sufficiently different from 0 ° to allow the 00 beam to hit the fluorescent screen. Figure 2 shows experimental (top curve) and theoretical (bottom curve) total elastic current calculated for constant $\beta = 0.25$ Ry and incident angles $\theta = 10$ ° and $\phi = 0$ °. The peak at approximately 45 eV is slightly less than 13% of the incident current in the experiment, while it is almost 20% in the theoretical current. In order to determine the value of $\beta$ that would match theory to experiment at this energy, we carried out calculations of the relative intensity $I/I_0$ at the same energy for a few different values of $\beta$, viz., in addition to 0.25 Ry, at 0.4, 0.5, and 0.75 Ry. The plot of $\log_{10}(I/I_0)$ vs $\beta$ in Fig. 3 reveals a linear dependence that allows easy interpolation to the value $\beta = 0.35$ Ry. The total elastic current calculated with this value of $\beta$ is compared to the experiment in Fig. 2 (middle curve). Now the whole theoretical curve is lower than before, as it should be, but quantitative agreement is only achieved at about 45 eV, where in fact $\beta$ has been determined to match the two curves. Clearly, better over-all quantitative agreement between

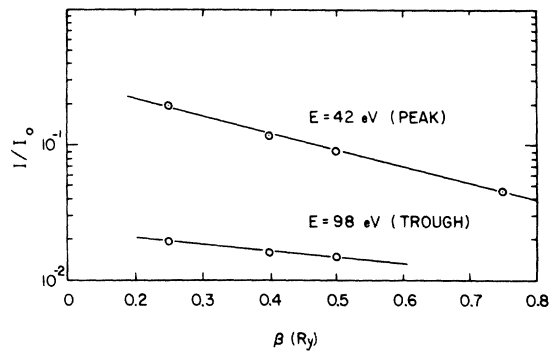


FIG. 3. Plot of $\log_{10}(I/I_0)$ calculated for different values of $\beta$ as a function of $\beta$ at two different energies.

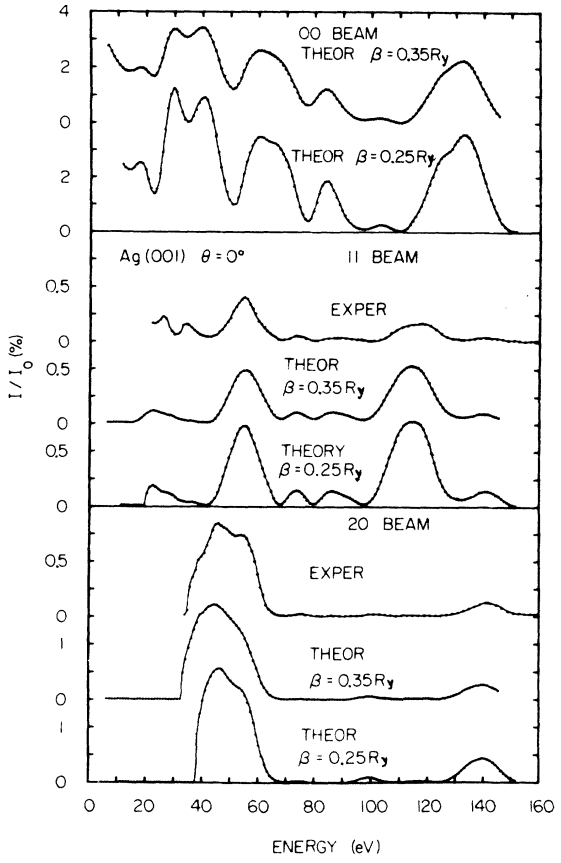


FIG. 4. LEED spectra from Ag{001} at normal incidence. Top panel: 00 beam, theoretical only ($\beta = 0.35$ Ry and $\beta = 0.25$ Ry). Middle panel: 11 beams, experimental and theoretical. Bottom panel: 20 beams, experimental and theoretical.

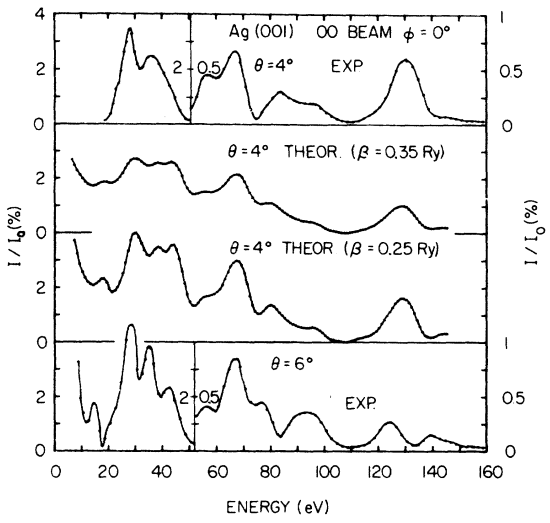


FIG. 5. LEED spectra from Ag{001}, 00 beam. Top: experimental ($\theta = 4°$, $\phi = 0°$). Middle: theoretical ($\beta = 0.35$ Ry and $\beta = 0.25$ Ry). Bottom: experimental ($\theta = 6°$, $\phi = 0°$).

theory and experiment can be achieved by fitting $\beta$ at a number of energies over the range investigated.

Before fitting a complete $\beta(E)$ curve we study how sensitive various features in the LEED spectra are to changes in the value of $\beta$ used in the calculations. Consider first the effect of a change in $\beta$ from 0.25 to 0.35 Ry (a 40% change) on individual beams at different angles. Figure 4 shows a few spectra at normal incidence: the specular beam (only theoretical) in the top panel, the 11 beam (fourfold degenerate) in the middle panel and the 20 beam (also fourfold degenerate) in the bottom panel. Beams are indexed on the basis of the face-centered net for fcc {001} surfaces as described, e.g., in Ref 1. We note that while all curves calculated with $\beta = 0.35$ Ry have lower intensities than those calculated with $\beta = 0.25$ Ry, the agreement with experiment remains highly satisfactory as far as peak shapes and positions are concerned. The same general conclusion may be drawn from Figs. 5 and 6, which concern the 00 beam at $\theta = 4°$ and $\theta = 10°$, respectively. Note that the agreement is much better at energies higher than about 50 eV for $\theta = 4°$ and higher than about 40 eV for $\theta = 10°$. However, comparison in the low-energy range between the theoretical curve calculated for $\theta = 4°$ and the experimental curve for $\theta = 6°$, and also between the theoretical curve at $\theta = 10°$ and the experimental curve at $\theta = 12°$, gives satisfactory agreement down

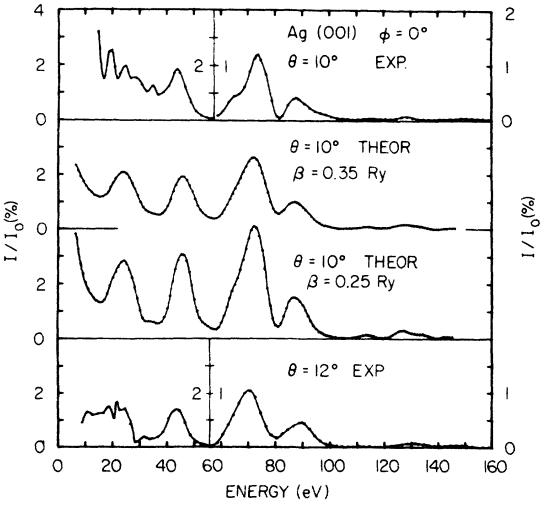


FIG. 6. LEED spectra from Ag{001}, 00 beam. Top: experimental ($\theta = 10°$, $\phi = 0°$). Middle: theoretical ($\beta = 0.35$ Ry and $\beta = 0.25$ Ry). Bottom: experimental ($\theta = 12°$, $\phi = 0°$).

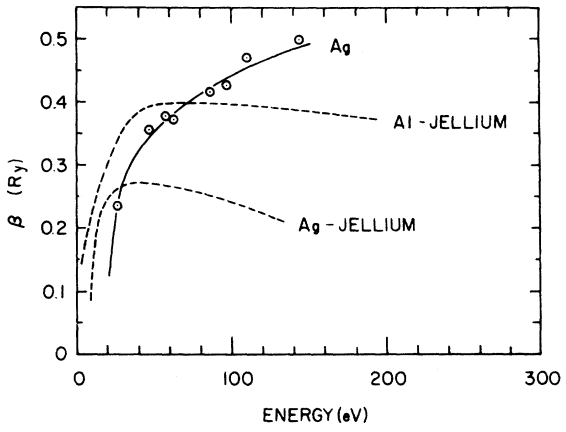


FIG. 7. Imaginary part $\beta$ of the scattering potential as a function of electron energy. Solid curve: result of fitting procedure described in the text. Dashed curves: results obtained from Lundqvist calculations for jellium (Ref. 19) adapted to aluminum and silver.

to energies of 20–30 eV. There appears to be a slow change in the angle of incidence in the experiment of the order of 2°, possibly owing to incomplete cancellation of residual magnetic (or electrical?) fields in the chamber. Although it is likely that the angle of incidence changed gradually over the range of energies investigated, it appears that the spectra can be subdivided in two portions: the range up to about 50 eV, in which the true angle of incidence is about 2° smaller than the quoted experimental angle, and the range above 50 eV, in which the quoted experimental angle is probably correct. With these qualifications it appears that over-all agreement in peak shapes and positions between theory and experiment is excellent. In terms of absolute intensities, the agreement is somewhat better in the range below 50 eV than in the range above 50 eV. However, as stated above, quantitative agreement in absolute intensities of individual beams is not likely to occur and is not expected if, as is commonly the case, the surface used in the experiment is not perfectly planar.

We can now proceed to determine the values of $\beta$ at a number of different energies so that the total elastic current calculated for a rigid lattice matches the total elastic current measured experimentally. To show that the linear relationship discovered in Fig. 3 for the plot of $\log_{10}(I/I_0)$ vs $\beta$ is not limited to intensity peaks, we have also drawn in Fig. 3 the corresponding data for 98 eV, where the total elastic current has a minimum, hence we use such linear plots to find $\beta(E)$. Thus the data for the total elastic currents calculated with $\beta = 0.25$ Ry and $\beta = 0.35$ Ry give a line for $\log_{10}(I/I_0)$ vs $\beta$ at each energy, which we use to pick the required $\beta$ to match theory and experiment at that energy. The result for $\beta(E)$ is shown in Fig. 7. The solid curve is drawn through the points determined by the above procedure; the dashed curves were obtained from Lundqvist's results for the imaginary part of the self energy of "jellium" crystals with the electronic densities of silver and aluminum, respectively (one electron per atom for silver and three electrons per atom for aluminum). It appears that at energies of about 20 eV the value of the imaginary part of the self energy for a real silver crystal is roughly one half that for silver jellium, while at about 140 eV the value for a real silver crystal is more than twice as large as that appropriate for a silver jellium. The two commonly used assumptions for the variation of $\beta$ with $E$ are that (i) $\beta$ is constant[3] and, (ii) $\lambda_{ee}$, the inelastic-collision damping length, is constant,[9] which corresponds to an $E^{1/2}$ dependence of $\beta$. Assumption ii corresponds more closely to the $\beta(E)$ in Fig. 7 than assumption i. However, except for the first experimental point at 26 eV (where the data are less reliable), the experimental values of $\beta$ fit an $E^{1/3}$ variation quite well.

The energy-dependent $\beta$ just determined has then been used to calculate the total elastic current (for the rigid lattice) at $\theta = 10°$ in order to test the quantitative agreement with experiment. Figure 8 shows that, in fact, such quantitative agreement, although not perfect, is reasonably satisfactory over the whole range of energies from about 20 to 140 eV.

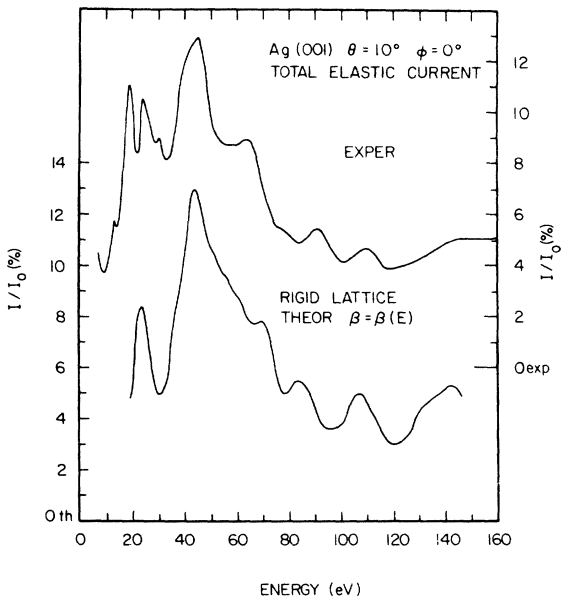


FIG. 8. Total elastic current reflected from Ag{001} at $\theta = 10°$, $\phi = 0°$. Top curve: experimental. Bottom curve: theoretical (rigid lattice, $\beta$ variable with energy as in Fig. 7).

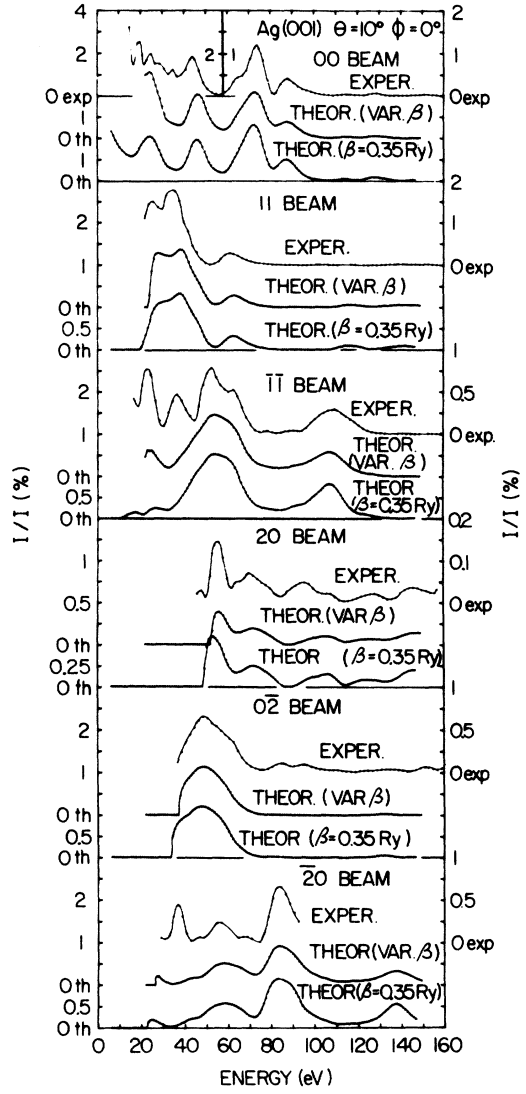


FIG. 9. LEED spectra from Ag{001} at $\theta = 10°$, $\phi = 0°$. The 11, $1\bar{1}$, and $0\bar{2}$ beams are each twofold degenerate. In each panel, the experimental curve is compared with two theoretical curves calculated with variable $\beta$ and constant $\beta = 0.35$ Ry.

### III. ANGULAR DEPENDENCE OF LEED SPECTRA

A complete set of nine beams for $\theta = 10°$ and $\phi = 0°$ is presented in Fig. 9 (each of the two 11-type beams shown and the $0\bar{2}$ beam are twofold degenerate) for the purpose of comparing experiment to calculations both with variable $\beta$ as determined above and with a constant $\beta = 0.35$ Ry. The qualitative agreement with experiment for both choices of $\beta$ is good at higher energies and the variable $\beta$ shows some improvement in shape matching even at lower energies (see, e.g., beam 11 below 50 eV), although for two beams, $1\bar{1}$ and to a lesser extent $\bar{2}0$, even the qualitative agreement is not satisfactory below about 60 eV. Before we examine whether the situation can be improved by taking into account the probable change in experimental incident angle that was discovered above, we consider the effect that a change in the surface potential barrier has on the calculated spectra.

Earlier calculations,[1] done with three different ways of matching waves at the surface, revealed some intensity changes but no great shape change of the spectra in the low-energy region. The simplest reasonable procedure, and the one that was adopted for all calculated spectra presented so far, is one that takes into account the refraction of the beams through the surface but eliminates the reflections in the potential step region (so-called "no-reflection" matching procedure). A physically more realistic model introduces a gradual potential change between vacuum and the crystal interior. A potential profile for the transition between crystal and vacuum was calculated by Lang and Kohn[21] using a semi-infinite uniform electron gas model (hence all quantities are constant in planes parallel to the surface); their result is approximated quite well by a hyperbolic tangent function $\tanh(z/d)$, with $d = 0.2a$, where $a$ is the lattice parameter 4.086 Å for silver. The resulting transition potential we call the Eckart-potential barrier, and we use the analytical solution of Eckart[22] for transmission through this barrier in the Ag calculation. In Fig. 10 we compare the 00 spectra at $\theta = 10°$ calculated with such an Eckart-potential barrier and with the usual no-reflection procedure. Except for the appearance (or, maybe, only the increase) of bumps around 33 and 52 eV, the Eckart-potential barrier does not seem to modify the spectrum very much. This statement holds true for a number of other spectra (not shown) at different angles. With one exception, to be discussed below, the adoption of an Eckart-potential surface barrier does not seem to improve the agreement between calculated and experimental data. For this reason, we will continue using the no-reflection matching procedure in the subsequent theoretical calculations.

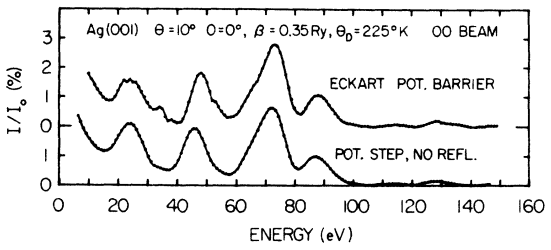


FIG. 10. Effect of surface potential barrier on LEED spectra of Ag{001}: 00 beam, $\theta = 10°$, $\phi = 0°$.

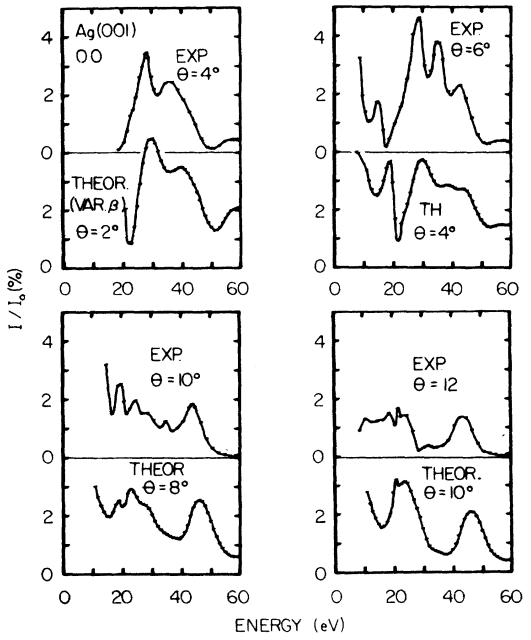


FIG. 11. LEED spectra from Ag{001} in the energy range up to 60 eV. The theoretical curves are all calculated for 2° less in $\theta$ than the labeled values of $\theta$ on the experimental curves.

The agreement seems to be consistently bettered, however, by taking into account the 2° discrepancy discussed earlier. Figure 11 shows comparisons in the energy range up to 60 eV between 00 spectra calculated with $\theta = 2°$, 4°, 8°, and 10° and 00 spectra measured with nominal $\theta = 4°$, 6°, 10°, and 12°, respectively. The qualitative agreement is good and the improvement over comparisons with data for the same nominal $\theta$ values is obvious. Similar conclusions may be drawn from Fig. 12 for the low-energy range of the nine nonspecular beams already examined in Fig. 9 for a nominal experimental $\theta = 10°$.

We now proceed to examine the ability of the theoretical calculations to reproduce experimental spectra at larger incident angles. Figure 13 presents the case of $\theta = 30°$, confirming the over-all good agreement with experiment and the improvement achieved by changing $\theta$ by 2°. Figure 14 gives the result for $\theta = 40°$ and indicates in addition an improvement in peak shapes (in particular, the bump around 42 eV) for a surface expanded by 5% with respect to simple termination of the bulk structure. Finally, for $\theta = 50°$ the results shown in Fig. 15 are much less satisfactory. The calculated spectra had to be displaced toward higher energies by 3 eV with respect to all other spectra examined above, and even the calculation with $\theta = 48°$ (or with an expanded surface, not shown) does not improve the agreement very much. The calculation done with an Eckart-potential barrier and constant $\beta = 0.25$ Ry seems to improve the situation at lower energies (appearance of small peak around 41 eV) but the large peak calculated around 70 eV is hardly visible in the experimental curve and the general trend above 80 eV is not very satisfactory. In view of the good agreement between theory and experiment obtained so far, and in view of the fact that the experimental data at these large incident angles must be collected "blindly" (i.e., without the help of the visual observation provided by fluorescent screen), it seems reasonable, in this case, to suggest the possibility of experimental error. The experimental curve could not be checked

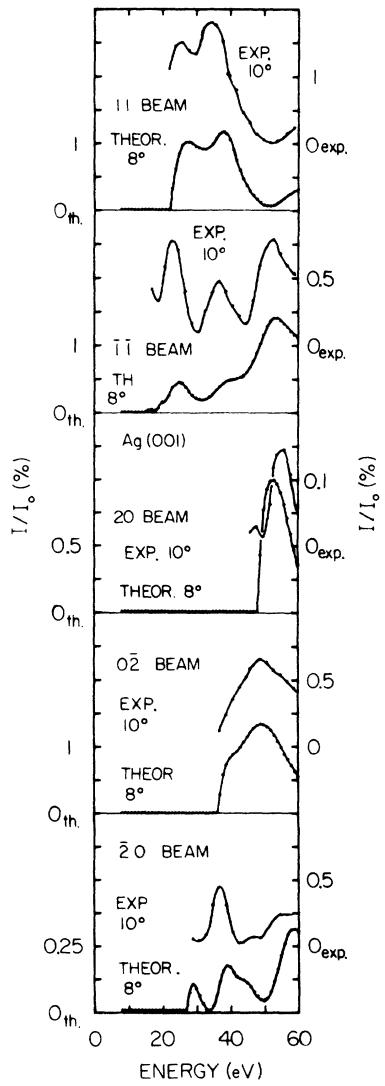


FIG. 12. Nonspecular LEED spectra in the energy range up to 60 eV from Ag{001} (compare with Fig. 9). Theoretical curves calculated for $\theta = 8°$, experimental curves reported for $\theta = 10°$.

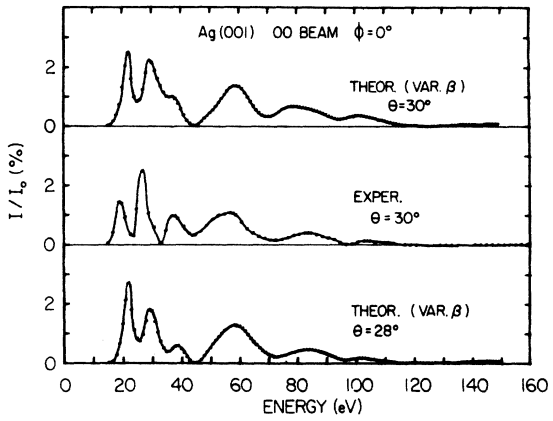


FIG. 13. LEED spectra from Ag{001}. Experimental curve (middle) for $\theta = 30°$, theoretical curves (top and bottom) for $\theta = 30°$, and $\theta = 28°$, respectively, and variable $\beta$.

because this discrepancy was discovered considerably after completion of the experimental run.

## IV. CONCLUSIONS

The present study demonstrates again that, as in the case of aluminum and copper, the layer-KKR method with band-structure potentials can give a good account of the LEED spectra of these pure close-packed metals, provided suitable corrections for lattice motion and inelastic scattering effects are introduced. With only one remaining uncertainty (at $\theta = 50°$) the theory reproduces peak positions, shapes and intensities equally well at high as at low angles of incidence. It appears, in fact, that the theory can detect discrepancies of at least 2° in the incident angles quoted in the experiment. Since the current quoted accuracy in angular resolution is ±2°, these results suggest that an improvement in this experimental parameter is desirable.

Quantitative agreement in absolute intensities between individual calculated and experimental beams is not attained and probably not attainable with "real" surfaces until and unless the effects of surface roughness can be conveniently introduced into and properly accounted for by the theoretical treatment. The procedure proposed in this paper provides a plausible way to determine the appropriate value of the imaginary part of the scattering potential from suitable experimental data. The accuracy of the assumptions that underlie the described procedure is however still to be established. Although the rough-surface scattering has the effect of transferring electrons from the beams into a diffuse background, just as the thermal and zero-point motion scattering do, some fraction of that diffuse background will be scattered into the crystal and lost. We assume that the fraction retained by the crystal is small. The procedure used for the lattice-motion effects, reported

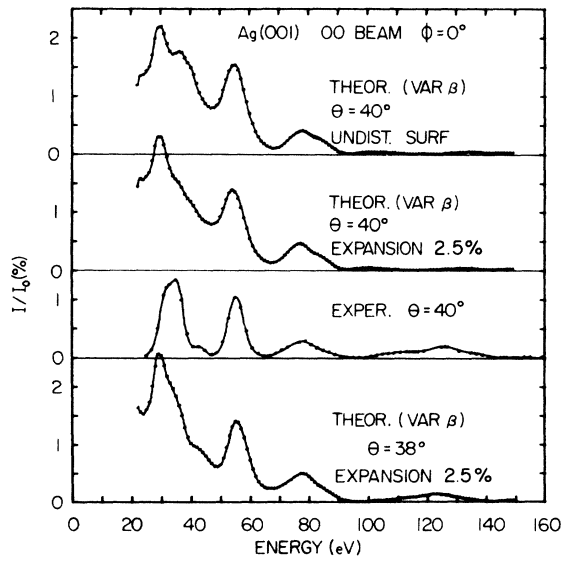


FIG. 14. LEED spectra from Ag{001}. Experimental curve (second from bottom) for $\theta = 40°$, theoretical curves calculated for abrupt termination of the bulk (top) and for surface expanded by 2.5% (second from top) at $\theta = 40°$, and for surface expanded by 2.5% at $\theta = 38°$ (bottom), all with variable $\beta$.

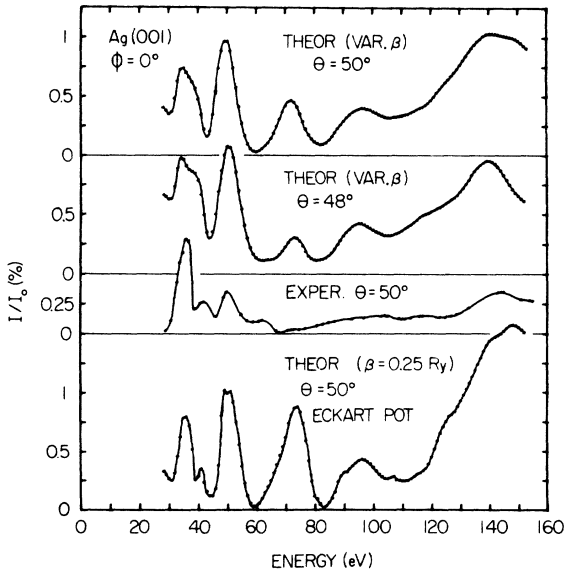


FIG. 15. LEED spectra from Ag{001}. Experimental curve (second from bottom) for $\theta = 50°$, theoretical curves calculated with variable $\beta$ for $\theta = 50°$ (top), $\theta = 48°$ (second from top), and with constant $\beta = 0.25$ Ry, for $\theta = 50°$ and Eckart potential barrier (bottom).

in a previous paper,[1] gives a prescription for defining complex phase shifts for an atom "blurred" in position by thermal motion. The total cross section for an atom given by these phase shifts can be split up using standard formulas into elastic and inelastic cross sections. We have assumed in this paper that electrons which are inelastically scattered in this way (quasielastic scattering) still come out of the crystal and contribute to the diffuse background. As in the case of roughness scattering, electrons which do not come out cannot be distinguished in the experiment from the electrons which suffer larger energy losses owing to the electron–electron scattering that is included in our formalism through the $\beta$ term. Hence, at worst, our procedure will give an upper bound for $\beta$. However it is encouraging that experimental tests of the small retention assumption, performed on silicon after this work on silver, indicate that the assumption appears to be quite adequate. These tests showed that the total elastic intensity scattered out of the crystal was not much changed by heating or by strongly disordering by ion bombardment; the details will be reported elsewhere.

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[1]D. W. Jepsen, P. M. Marcus, and F. Jona, Phys. Rev. Lett. **26,** 1365 (1971); Phys. Rev. B **5,** 3933 (1972).
[2]P. M. Marcus, D. W. Jepsen, and F. Jona, Surf. Sci. **31,** 180 (1972).
[3]D. W. Jepsen, P. M. Marcus, and F. Jona, Phys. Rev. B **6,** 3684 (1972).
[4]D. W. Jepsen and P. M. Marcus, *Computational Methods in Band Theory* (Plenum, New York, 1971), p. 416.
[5]C. B. Duke and G. E. Laramore, Phys. Rev. B **2,** 4765 (1970).
[6]G. E. Laramore and C. B. Duke, Phys. Rev. B **2,** 4783 (1970).
[7]F. Jona, D. W. Jepsen, and P. M. Marcus, Sixth LEED Seminar, Washington, D. C., April, 1972 (unpublished).
[8]C. B. Duke, in *LEED: Surface Structure of Solids*, edited by L. Laznicka (Union of Czechoslovak Mathematicians and Physicists, Prague, Czechoslovakia, 1972), pp. 124 and 361.
[9]G. E. Laramore and C. B. Duke, Phys. Rev. B **5,** 267 (1972).
[10]S. Y. Tong and T. N. Rhodin, Phys. Rev. Lett. **26,** 711 (1971).
[11]G. E. Laramore, C. B. Duke, A. Bagchi, and A. B. Kunz, Phys. Rev. B **4,** 2085 (1971).
[12]J. B. Pendry, J. Phys. C **4,** 2514 (1971).
[13]G. E. Laramore, J. Vac. Sci. Technol. **9,** 625 (1972).
[14]E. W. Hu, R. M. Goodman, and F. Jona, preceding paper, Phys. Rev. B 8, 5569 (1973) (referred to as I).
[15]E. C. Snow, Phys. Rev. **172,** 708 (1968).
[16]J. F. Janak, Solid State Commun. **10,** 833 (1972).
[17]D. W. Jepsen, P. M. Marcus, and F. Jona, Surf. Sci. **39,** 27 (1973); see also Ref. 7.
[18]M. G. Legally, Z. Naturforsch. A **25,** 1567 (1970).
[19]G. E. Laramore, J. E. Houston, and Robert L. Park, J. Vac. Sci. Technol. **10,** 196 (1973).
[20]B. I. Lundqvist, Phys. Status Solidi **32,** 273 (1969).
[21]N. D. Lang and W. Kohn, Phys. Rev. B **1,** 4555 (1970); Phys. Rev. B **3,** 1215 (1971).
[22]C. Eckart, Phys. Rev. **35,** 1303 (1930).