Comparison of Model Calculations of Low-Energy-Electron-Diffraction Intensities from Be(0001) and Al(001)†

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Low-energy-electron-diffraction (LEED) intensity profiles are calculated using the phenomenological s-wave inelastic-collision model for electrons incident on Be(0001) and Al(001). The predicted intensity profiles are compared both with those obtained in two recent calculations (performed using "realistic" potentials) and with experimental data. When strong inelastic-collision damping is included in the model, the correspondence between the two types of calculations is comparable to that between either of the calculations and the experimental data. This result remains valid over wide ranges of values of the parameters used in the inelastic-collision model. It reflects an insensitivity of certain qualitative features of the model predictions to the values of the "material" parameters used in the calculation. This insensitivity is fortunate because an examination of the realistic potential models suggests that they fail to consider several surface and many-body phenomena which seem to be of significance in determining the intensity profiles.

I. INTRODUCTION

As evident from two recent letters on Be(0001)[1] and Al(001),[2] model calculations of low-energy-electron-diffraction (LEED) intensity profiles are becoming sufficiently refined to permit direct comparison with experimental data.[1-12] The most adequate models[1-6,8-11] treat the electron as moving both in a static periodic potential (which, e.g., presumably describes the Fermi surface of a metal target) and in a complex energy-dependent potential which simulates the consequences of electron-electron interactions.[13-15] However, a central issue, currently under discussion,[1,2,6,8-10,16-19] is whether or not such a model provides an adequate (i.e., "realistic") theoretical description of the phenomenon of LEED. In particular, it is our view that such models exhibit substantial conceptual difficulties associated with their neglect of surface many-body effects[6,14,17,19,20] and (high-energy) electron-electron interaction-induced vertex corrections.[19] These difficulties prohibit the models from providing a realistic description of LEED in the same sense that they are known to provide an excellent quantitative description of the bulk low-temperature properties of metals.[21] It is our purpose in this paper to consider the extent to which results comparable to those of the above-mentioned calculations[1,2] are predicted by the phenomenological s-wave inelastic-collision model.[6,9,10,14] We also examine, in these two cases, some selected aspects of the sensitivity of the predictions of this model to the values of the parameters characterizing the electron-solid interactions. By comparing the model calculations, both to each other and to experimental data, we achieve insight into the uniqueness of various features of the model predictions and into the adequacy of these models for the description of the observed phenomena.

We proceed in two steps. In Sec. II we enumerate and document the conceptual difficulties inherent in conventional static-potential models which have been advanced as indicating their inadequacy as the basis of a quantitative description of LEED. In Sec. III we present the results of the inelastic-collision-model calculations. The significance of these results is discussed in the light of the remarks in Sec. II. Finally, our main conclusions are summarized in Sec. IV.

II. OBSERVATIONS ABOUT STATIC-POTENTIAL MODELS

As this paper contains the presentation of alternative calculations of LEED intensities from Be(0001) and Al(001), a logical initial task is the discussion of the issues involved in the construction of the models which underlie these calculations. This discussion serves two purposes. First, in comparing the results of calculations based on different models it is necessary to have some perspective, provided in this section, on the significance of the distinctions between the models. Second, in Refs. 1 and 2 the appellation realistic

is applied to the potential[1] and calculation,[2] respectively. As our model and those used by the authors of these references emphasize different aspects of the physical process of electron-solid scattering, it is informative to sharpen our definition of the ingredients of a model of this process which could be regarded as realistic in the same sense as similar models of the bulk properties of solids.[21] Investigations of the quantitative consequences for the predicted LEED intensities of various refinements to the initial model calculations are just beginning.[6,8-10,16-20,22-25] However, estimates of the qualitative nature and sometimes the magnitude of these consequences are available currently. Such estimates provide a useful guide for comparing the various calculations to each other, and for assessing the significance of their points of agreement with experimental measurements.

Any model of LEED from solid surfaces must either explicitly or implicitly deal with three phenomena which are not important for the calculation of the properties of bulk solids via energy-band theory: the induction of surface charge on the solid by the incident electrons, the high energies (relative to the Fermi energy) of these electrons, and the sensitivity of the elastic scattering cross sections to the specifically surface properties of the solid (caused by the rapid attenuation of the elastic-wave field in the solid due to inelastic collisions). We proceed by examining the description of each of the these phenomena by current static-potential models.

We define a "static-potential model" to be one in which the electronic eigenstates are obtained via a self-consistent solution to the Hartree-Fock approximation to the Schrödinger equation for the motion of electrons in the Coulomb field of a fixed array of ion cores. As the actual calculations[1-12] have not thus far achieved this ideal, one must distinguish between the consequences of their failure to be truly self-consistent solutions to the Hartree-Fock equations and the consequences of the use of the Hartree-Fock approximation *per se*.

In existing model calculations,[1-5,7,8,12,26-30] the evaluation of the LEED intensity profile is decomposed into two steps. First, a model one-electron potential is determined by an appropriate approximate solution to the Hartree-Fock equations in a bulk solid. Next, the LEED boundary-value problem is solved either by using directly a truncated version of this potential or by joining the wave functions outside a planar crystal face to appropriate linear combinations of the Hartree-Fock wave functions inside via continuity of the wave function and its derivative at the planar interface. In these calculations, electron-electron-induced damping of the elastic-wave field is either ignored[2,7,12] or taken into consideration by the addition of a complex optical potential to the crystalline potential inside the solid.[1,3-6,8-11,13-15] Therefore all these models exhibit three important features: (i) Vibrational motion of the ion cores is neglected; (ii) the potential is that characteristic of a truncated but otherwise periodic bulk solid; (iii) the potential is evaluated, at best, in the Hartree-Fock approximation or a further approximation thereto.

From the considerations of the previous paragraph we see that none of the static-potential calculations are based on models which describe the consequences either of the induced surface charge[31-36] or of the vertex corrections to the elastic electron–ion-core scattering amplitudes caused by the electron-electron interactions (in particular by plasmon emission and reabsorption[19]). Only a few calculations[8,22-24,37] consider the effects of the geometrical inequivalence of the surface and bulk layers, a few[6,9,10,37] the effects of their electronic inequivalence, and only one[17,18] the effects of their vibronic inequivalence. Therefore two questions arise naturally. How substantial are the consequences of these phenomena? To what extent do the model calculations described herein constitute an improved treatment of them?

Estimates of the magnitude of the effects of the various phenomena as found in the literature may be summarized as follows. Considering first the consequences of induced surface charge, comparison of LEED intensities calculated using a truncated image potential with those calculated using a step-well potential to describe the inner potential in a one-dimensional model indicates that even for energies ten times higher than the inner-potential shift the predicted intensities from the truncated image potential are between a factor of 2 and 10 lower than those from the step well.[22] This result is in agreement with the assertion of Strozier and Jones[1] that the absolute intensities are sensitive functions of the potential, but does not promote confidence in the ability of existing static-potential models to predict these intensities accurately. However, the influence of induced surface charge may not be so severe at high electron energies (i.e., energies well above the surface-plasmon energy) because the image potential is the low-energy limit of virtual surface-plasmon creation.[38] For electron energies above the surface-plasmon threshold, the electron fluid in the solid cannot respond as effectively to the incident electron and the real part of the ("image") potential due to the induced surface charge is reduced substantially.[38] The plasmon-exchange vertex corrections to the electron–ion-core elastic-scattering amplitudes have been estimated by Duke and Laramore,[19] who found them to be comparable to the bare scattering amplitudes and sensitive to the values of the parameters of the incident beam. Calculations[22-25] of the consequences of a rigid expansion of the outer layer indicate that

reasonable values of the expansion (i.e., 5–10%) cause only a small effect on the lower-energy ($E \lesssim 100$ eV) intensity profiles for normal incidence. However, such an expression exerts a marked influence on the dependence of the structure near a kinematical Bragg peak on the angle of incidence of the electron beam and, at low temperatures, on the intensity of this structure near normal incidence at high energies.[37] An analysis[18] of the influence of the vibronic inequivalence of the surface and bulk layers led to the conclusions that this inequivalence reduces the effective scattering amplitude from the surface layer (usually making the intensity profiles more kinematical in appearance)[6,9,10,18,37] and causes the magnitude of the peak(s) near the kinematical Bragg energies to diminish more rapidly with increasing temperature.[18,37] Finally, studies[6,9,10,18,37] of the consequences of the electronic inequivalence of the surface and bulk layers indicate that the predicted intensity profiles are sensitive to this inequivalence primarily when it is small. If the surface layer(s) scatters much less strongly than the bulk, the intensity profiles become kinematic in appearance. If it scatters more strongly than the bulk, complicated profiles result which, however, are relatively insensitive to further minor variations in the model parameters.

The literature survey sketched above reminds us of one central fact. All static-potential models, no matter how refined, tend to describe only one aspect of the electron-solid scattering problem, the construction of the electron–ion-core scattering amplitude for "bulk" ion cores, very accurately. However, they either neglect or describe crudely the effects of induced surface charge, electron-electron vertex renormalization, electron-phonon vertex renormalization, and the specifically surface aspects of the electron-ion interactions. The model calculations presented in Sec. III are in no essential way any more refined than others in the literature.[1–12,18,26–30] On the contrary, they are based on a much less-refined model of the bare electron–ion-core potential than that which underlies either of the calculations to which they are compared.[1,2] The result which we wish to establish herein is the existence of certain "universal" qualitative features of all model calculations with strong electron–ion-core scattering and strong inelastic-collision clamping. This conclusion originally was reached and documented in a long paper submitted some time ago.[10] However, the subsequent appearance of Refs. 1 and 2 led us to analyze Be(0001) and Al(001) in detail. Our main task in Sec. III is to demonstrate that measured in terms of describing the qualitative features of experimental LEED intensity profiles, a variety of model calculations provide comparable results in these cases also. Viewed in the light of the considerations given above, this result has two nontrivial consequences. First, it provides a sound basis for the hope[9,10,14,39–41] that despite the host of difficulties inherent in the construction of a completely satisfactory microscopic theory of LEED, model calculations of the type described both herein and in Ref. 1 can achieve the more modest goal of the extraction of geometric-structure information from experimentally measured LEED intensities. Second, it suggests that as for the purpose of structure analysis a detailed model of the electron-solid potential seems to be unnecessary. Therefore, simple empirical models, like the one described herein, may suffice for this application. This is an important conclusion because the construction of an accurate description of the electron-solid interaction appears rather hopeless in most cases of practical interest from the point of view of structure determination[39–41] (e.g., the surface crystallography of chemisorbed monolayers and multilayers).

Summarizing, semiquantitative or quantitative descriptions of the intensity profiles over wide ranges of the energy and direction of the incident beam undoubtedly cannot be achieved without an accurate description of the electron-solid interaction. References 1 and 2 are attempts to provide such a description of the short-range low-energy part of this interaction. The major result of our consideration in this section is the recognition that a realistic determination of this part of the interaction alone need not suffice to provide a realistic (i.e., semiquantitative) description of experimental LEED intensities. The main result of our considerations in Sec. III is the demonstration that for Be(0001) and Al(001) a detailed knowledge of this short-range part of the interaction is sufficient but not necessary to achieve a qualitative description of the intensity profiles. This demonstration is significant because it implies that crude models of the electron-solid interaction may suffice for the purpose of geometric-structure determination in cases for which an accurate description of the interaction is either impractical or impossible.

III. PRESENTATION OF RESULTS

A. Definition of Model

All of the results presented in this paper were obtained using the matrix-inversion analysis of the phenomenological s-wave inelastic-collision model as described by Tucker and Duke.[10] This model is characterized by four parameters. The average real electron-electron–induced electronic self-energy (inner potential) is taken to be a constant denoted by $-V_0$. The inelastic-collision-model damping is described by an electronic mean free path λ_{ee} which is predicted[9,14] to be nearly constant, $4 \lesssim \lambda_{ee} \lesssim 8$ Å, for incident-electron energies in the range $50 \lesssim E \lesssim 200$ eV. Our values of λ_{ee} at lower

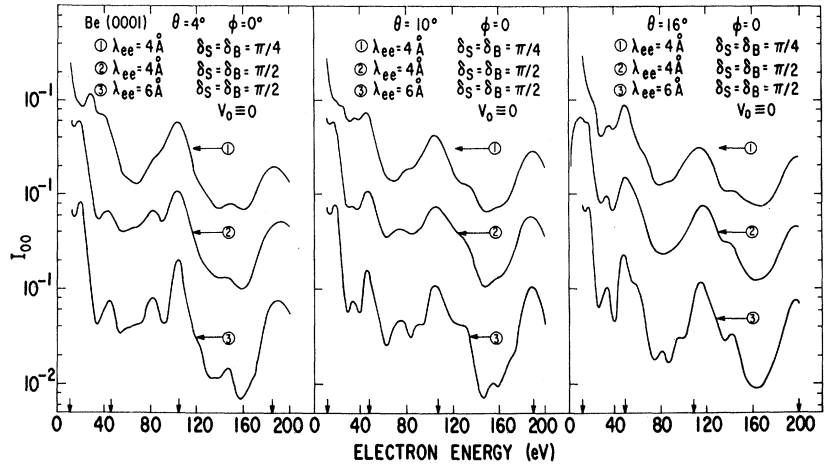

FIG. 1. Intensity profiles for the (00) beam of electrons scattered from Be(001) for various angles of incidence. The incident beam lies in a plane determined by the normal to the surface and a line between two adjacent atoms. The calculations were performed using the matrix-inversion analysis described in Ref. 10 using the parameters indicated in the figure. The lattice parameters of Be were taken to be $a_0 = 2.283$ Å and $c_0 = 3.607$ Å. The arrows at the bottom of each panel designate the energies of the kinematic primary Bragg maxima.

energies are less realistic than those used by Strozier and Jones[1] but, as noted in Sec. II, suffice for our present purposes. Finally, the electron-ion-core scattering is expressed in terms of a (single) s-wave phase shift δ for electron–ion-core scattering. We consider the surface layer of scatterers to be characterized by a phase shift δ_S which need not be identical with that, δ_B, of the other "bulk" ion cores. In any direct analog of both of the calculations[1,2] to which we compare our results, $\delta_S = \delta_B$ by construction. For simplicity we take both δ_S and δ_B to be independent of energy: an approximation which, like the s-wave model itself, is "unrealistic" but is useful in permitting us to examine the sensitivity of the predicted intensity profiles to the values of the model parameters.

B. Be(0001)

Our discussion of this case is based on an investigation of the extent to which the extremely simplified phenomenological s-wave inelastic-collision model reproduces the results of the microscopic (second-order perturbation-theory) calculations of Strozier and Jones.[1] As these authors (arbitrarily) set the real part of the proper self-energy equal to zero, we take $V_0 \equiv 0$. In their calculation the use of the "bulk-scatterer" potential form factors requires $\delta_S = \delta_B = \delta$. In Fig. 1 we show the inelastic-collision-model predictions for strong ($\delta = \frac{1}{2}\pi$) and moderate ($\delta = \frac{1}{4}\pi$) scattering. Note the prominence of structure near the kinematical Bragg positions in all of the calculations. Results for both $\lambda_{ee} = 4$ and 6 Å are shown because comparison of the scale of the fine structure in the model predictions with the data of Baker[42] as quoted by Strozier and Jones[1] indicates that, as expected,[9,14] this is the range of values of λ_{ee} which is appropriate to describe the data. Comparison of Fig. 1 with Baker's data indicates that the structure in it near 80 eV is associated with the interlayer multiple-scattering peaks (ILMSP's) near the $n = 3$ Bragg energy whereas that between 160–180 eV is associated with the ILMSP's near the $n = 4$ Bragg energy. This observation is also consistent with Strozier and Jones's calculations.

In order to examine the sensitivity of the model predictions to the relative strengths of the surface and bulk electron–ion-core scattering potential, we calculated the intensity profiles associated with various values of δ_S and δ_B as discussed by Duke and Tucker.[6,10] Some typical results are shown in Fig. 2. As described earlier,[6,10] structure near

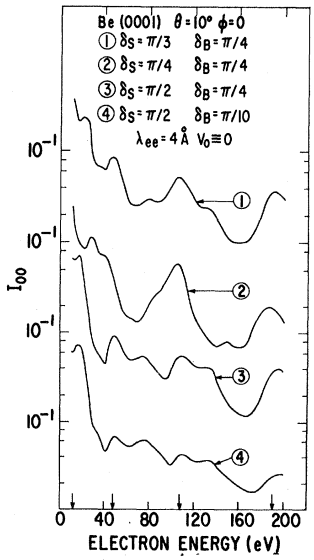

FIG. 2. Intensity profiles for the (00) beam of electrons scattered from Be(0001) for a 10° angle of incidence. The plane of incidence and lattice parameters of Be are identical to those used in determining Fig. 1. The calculations were performed using the matrix-inversion analysis (Ref. 10) for the parameters indicated in the figure. Arrows designate the energies of the kinematic primary Bragg maxima.

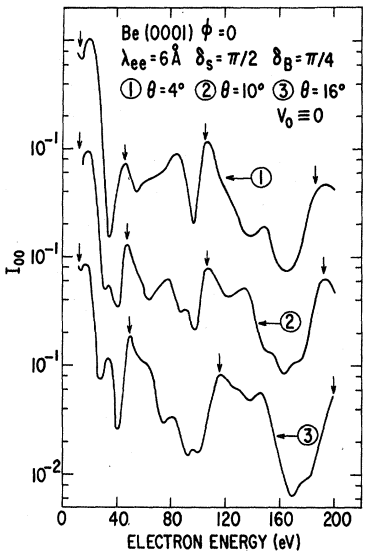

FIG. 3. Intensity profiles for the (00) beam of electrons scattered from Be(0001) at various angles of incidence. The plane of incidence and lattice parameters of Be are identical to those used in determining Fig. 1. The calculations were performed using the matrix-inversion analysis (Ref. 10) for the parameters indicated in the figure. Arrows designate the energies of the kinematic primary Bragg maxima.

the Bragg energies remains prominent, but setting $\delta_B \ll \delta_S$ causes a substantial enhancement of the ILMSP's between the Bragg energies. This is particularly evident from curve 4 in Fig. 2 for which the ILMSP at 76 eV is comparable in intensity to the $n=2$ Bragg resonance and more intense than the ILMSP structure at the $n=3$ Bragg energy. This behavior contrasts sharply to that shown in curves 1 and 2 in the figure for which $\delta_S \leq \delta_B$. Correspondence with Baker's results suggests that the 80-eV ILSMP is associated with the peak in his ($\theta=30°$) data near 50 eV. Strozier and Jones also get a strong peak at this energy with their bulk potential. In fact, curves 3 and 4 in Fig. 2 compare as favorably to Baker's data as do Strozier and Jones's results. This fact becomes even more evident if we use $\lambda_{ee}=6$ Å, the consequences of which are shown in Fig. 3, in order to enhance the appearance of fine structure in the predicted profile. Indeed, if, following Fig. 2 in Strozier and Jones,[43] we choose $V_0 \cong 28$ eV to line up the resonances near the $n=4$ Bragg energy, then we obtain a one-to-one correspondence between *all* of the fine structure in curve 2 in Fig. 3 and that in Baker's data. This result is evident from Fig. 4 in which we compare our calculated values to Baker's data at all three angles $\theta=4°$, 10°, and 16°. The only discrepancy at $\theta=10°$ is our failure to predict any fine structure near 90 eV. A similar remark holds for the $\theta=4°$ data using $V_0=20$ eV. (In this case we fail to predict the observed fine structure only near 150 eV.) The $\theta=16°$ case is our worst one. In order to get the ILMSP near 112 eV to line up with the experimental peak near 80 eV we need an inner potential of $V_0=32-34$ eV. The structure below 80 eV correlates well with Baker's data but the intensities above this energy are predicted to be too large for the values of the model parameters used in constructing Figs. 3 and 4. The least satisfactory aspect of the results shown in Fig. 4 is our use of an angular-dependent inner-potential shift. Even in Strozier and Jones's analysis the details of this feature of the calculation are unclear.[43] Baker[42] indexed his data using an average inner potential of 22 eV. Both model calculations clearly display the predominance of structure near the kinematical Bragg energies (i.e., $\pm\sim 5$ eV) in agreement with the data for an inner potential $V_0\sim 25$ eV.

In summary, we have devoted essentially no effort to optimizing the parameter choice in our model calculation. Yet our model description of Baker's data is comparable to that achieved by Strozier and Jones, after considerably more labor expended to evaluate the electron–ion-core potential

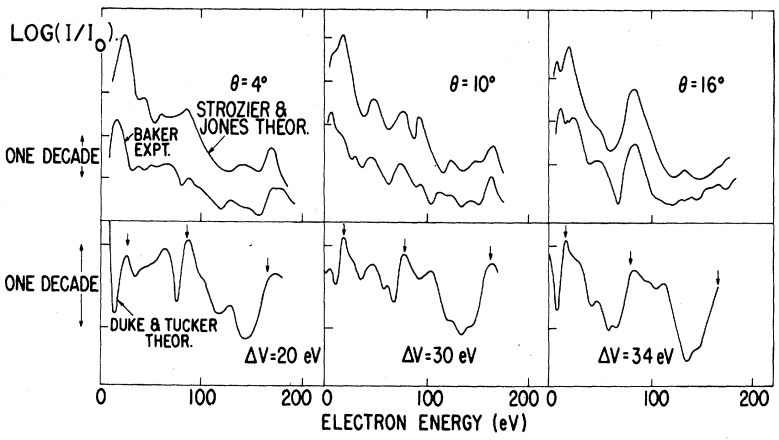

FIG. 4. Comparison of experimental and calculated intensity profiles for the (00) beam of electrons scattered from Be(0001) at various angles of incidence. The top two panels are taken directly from Fig. 2 of Ref. 1. The lower panel is obtained by shifting (by ΔV) the voltage axis of the curves shown in Fig. 3. The parameters used in the calculation are $\delta_S=\frac{1}{2}\pi$, $\delta_B=\frac{1}{4}\pi$, and $\lambda_{ee}=6$ Å.

in their microscopic realistic model. (For example, our predictions of the peak positions are visibly better at $\theta = 4°$, the two are comparable at $\theta = 10°$, and theirs is visibly better at $\theta = 16°$.) Both model calculations contain adjustable inner-potential corrections. Our analysis is not particularly sensitive to the damping parameter if we use values in the physically sensible range.[9,14,15] By making the damping increase with increasing energy according to the jellium model[9] we can describe the drop in intensity at low voltages better than the single-parameter results shown in the figures.[9] The sensitivity of the results to the phase shifts is displayed explicitly in Figs. 1 and 2. One finds satisfying Strozier and Jones's result that an approximate analysis based on a reasonable microscopic model gives a description of most of the main features of Baker's data. However, a qualitative description of these features is clearly not unique. Doubtless the microscopic model calculations will be improved still further.[44] Possibly the difficulties noted in Sec. II can be overcome. However, we think our analysis reveals that the predominance of structure near the kinematical Bragg energies is a reliable systematic prediction of a variety of models, and consequently provides a suitable abstraction from these models for use in surface crystallography.[10,16] It also reveals that qualitative descriptions of Baker's data, comparable to that achieved by Strozier and Jones,[1] are not too difficult to achieve. Therefore, this accomplishment does not constitute an adequate figure of merit for the precision of microscopic model. A realistic model in the sense discussed in Sec. II must predict both the absolute magnitude and the fine details of the intensity profiles with no adjustable parameters (especially inner potential shifts) at all. The phenomena involved can be subtle surface and many-electron effects. Therefore, we regard the construction of such a model to be more difficult than that of the conventional static-potential models.

C. Al(001)

As detailed inelastic-collision-model analyses of elastic scattering from Al(001) have been performed using both perturbation theory[37,44,45] and matrix inversion,[37,44,46] we confine our attention to comparison of some of the salient features of a matrix-inversion calculation with those of the calculation performed by Hoffstein and Boudreaux.[2]

The essential feature of elastic scattering from Al(001) is that for bombarding energies above about 30 eV, the main features of the intensity profiles are predicted by the kinematical model. This fact is true both experimentally[7,47,48] and theoretically.[6,10,40,45,46] This result is predicted by the s-wave inelastic-collision model for a wide variety of values for both δ_S and δ_B. Taking $\delta_S = \delta_B = \delta$ for compatibility with Hoffstein and Boudreaux's "bulk" potential, our model predictions for intermediate-strength scatters ($\delta = \frac{1}{4}\pi$) are compared with theirs and with the experimental data in Figs. 5 and 6 for the (00) and (11) beams, respectively [Jona[48] labels our (11) beam[10] as the "20" beam due to his use of a nonprimitive surface unit cell]. These figures illustrate the excellent description of the qualitative features of experimental data afforded by the s-wave inelastic-collision model using the intuitively obvious parameters $V_0 = \zeta + \phi = 16.7$ eV and $4 \lesssim \lambda_{ee} \lesssim 8$ Å. The quantity ζ is the Fermi energy for a free-electron gas of the density of aluminum and ϕ is the work function of Al(100). As we have emphasized earlier,[40] a kinematical indexing procedure works flawlessly for large peaks in all of the beams associated with Al(001). Thus we see that as anticipated,[14] the strong inelastic-collision damping has restored the validity of the kinematical indexing of the major peaks in the data despite the dynamic character of the peaks as clusters of ILMSP's near the Bragg energies.[10] Indeed the nature of these peaks as broadened clusters of ILMSP's is evident immediately from Hoffstein and Boudreaux's analyses as well as those of Morse[49] and ourselves.[10]

IV. CONCLUSIONS

From the discussion given in Sec. II, we conclude that an adequate model for a quantitative description

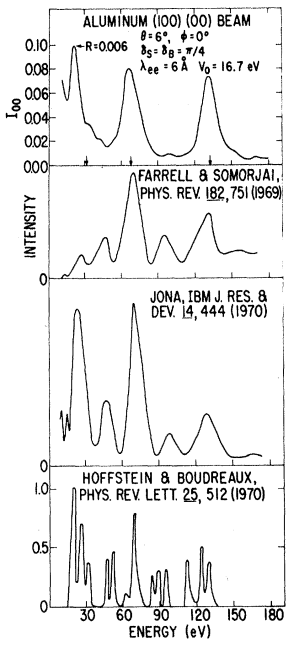

FIG. 5. Comparison of experimental and calculated intensity profiles for the (00) beam of electrons scattered from Al(001) for a 6° angle of incidence in the plane determined by the normal to the surface and a vector between two nearest-neighbor surface atoms. (We follow the notation of Refs. 2 and 10 rather than Ref. 48.) The lower three panels are Fig. 2 in Ref. 2. In the upper panel is shown the intensity profile calculated using the matrix-inversion analysis (Ref. 10) for the parameters indicated in the figure. Arrows designate the energies of the kinematical primary Bragg maxima. The magnitude of the maximum reflection coefficient (of 0.6%) is indicated in the figure for comparison with the calculations of Hoffstein and Boudreaux (Ref. 2) shown in the bottom panel.

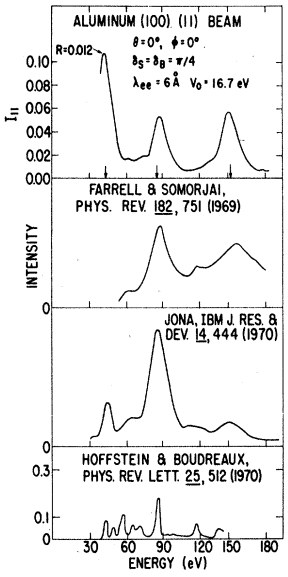

FIG. 6. Comparison of experimental and calculated intensity profiles for the (11) beam of electrons scattered from Al(001) for normal incidence ($\theta = \phi = 0$). The lower three panels constitute Fig. 3 in Ref. 2. In the upper panel is shown the intensity profile calculated using the matrix-inversion analysis (Ref. 10) for the parameters shown in the figure. Arrows designate energies of the kinematical primary Bragg maxima. The magnitude of the maximum reflection coefficient (1.2%) is indicated in the figure for comparison with the calculations of Hoffstein and Boudreaux shown in the bottom panel.

of LEED intensity profiles either must incorporate treatments of the induced "image" charge, modified ion-core screening at the surface, surface lattice-parameter changes, zero-point vibrational motion of the ion cores, off-diagonal contributions to the electron inner potential (i.e., a nonlocal propagator renormalization), and dynamic electron-electron-induced vertex corrections to both the electron-electron and electron–ion-core interactions, or demonstrate that their consequences are negligible. As the existing (static-potential) model calculations do not deal with these topics, we reexamined the description of experimental data by two recently published calculations.[1,2] We found that without any effort at parameter optimization, the phenomenological s-wave inelastic-collision model[6,9–11] provides a comparable description of the qualitative features of the data. From this result we conclude that in the strong-damping moderate-scattering limit, the geometry of the lattice rather than the dynamic nature of the electron-solid potential dominates the qualitative features (as opposed to quantitative details) of the intensity profiles. As anticipated from the discussion in Sec. II, none of the calculations describe adequately the detailed structure in the experimental intensity profiles. However, as described earlier in other cases[10,40] for Al(001) and Be(0001), the s-wave inelastic-collision model describes the data with sufficient accuracy to extract the gross geometric structure of the target.

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[44]Substantial progress in this endeavor has been achieved since the submission of this manuscript. Results on Al(100) have been reported at the 1971 LEED Seminar by Marcus and Jepson, Tony and Rhodin, Strozier and Jones, and Duke, Laramore, and Tucker. Calculations on the nonspecular beams of Be(0001) were reported by Strozier and Jones and by Zimmer, and on Al(111) and Al(110) by Duke, Laramore, Holland, and Gibbons. These analyses reveal that using an improved electron-ion-core potential materially improves the description of data for small angles of incidence and intermediate energies ($20 \leq E \leq 200$ eV). The description of data at low energies and large ($\theta \gtrsim 15°$) angles of incidence remains qualitative in nature.
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Anharmonic Interactions in Aluminum. II

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Additional calculations of the one-phonon spectral function in aluminum are presented. Results are given in the temperature range $300 \lesssim T \lesssim 900$ K for phonons propagating along the symmetry directions [100], [110], [111], and [310]. The frequency shifts and linewidths of the [310] phonons are compared with the high-temperature neutron scattering data of Larsson *et al.* In addition, for those phonons whose resonance shapes develop prominent structure, the spectral functions are explicitly displayed and discussed.

I. INTRODUCTION

In a previous paper[1] anharmonic linewidths and frequency shifts were calculated for aluminum at the two temperatures 80 and 300 K for phonons propagating along the [100], [110], and [111] symmetry directions. Agreement with the available experimental neutron scattering data was satisfactory. The calculation was based on a model pseudopotential whose parameters were determined so as to reproduce the experimental phonon dispersion curves in aluminum at 80 K.

The present work extends the calculations of I to higher temperatures. The approximations involved are the same as were discussed previously. In the treatment of I, only the lowest-order anharmonic corrections to the phonon self-energy were included, i.e., the quartic interaction to first order and the cubic interaction to second order. Since the Debye temperature of aluminum is ~ 400 K, we might expect that the neglect of anharmonic interactions of higher order (e.g., four-phonon decay processes) would introduce quantitative errors for $T \gg \Theta_D$. In order to obtain a partial assessment of the importance of the higher-order anharmonic corrections, calculations of frequency shifts and linewidths were carried out for selected [310] phonons and comparison made with the high-temperature neutron data of Larsson *et al.*[2] Satisfactory agreement was found for the over-all trends with temperature of the frequency shifts and linewidths over the range of temperatures considered. The large ex-