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EXPTL

THEORET~~ICAL~~ AND EXP~~ERIMENTAL~~ INVEST~~IGATIONS~~ OF THE PHYS~~ICS~~ OF CRYSTALLINE SURFACES

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I. SUMMARY OF WORK

The efforts during the first year were concentrated on the first part of the problem as defined in the research proposal, i.e. on

(1) the influence of the interface on the epitaxial growth of thin films and

(2) the characterization of surfaces.

The work falling into category (1) can be divided up in the following way:

(1a) theoretical work on interfacial energy and nucleation;

(1b) the growth of f.c.c. metals on alkali halides in ultrahigh vacuum (UHV) using UHV grazing incidence electron diffraction, mass spectrometry, conventional electron microscopy and transmission electron diffraction as experimental tools;

(1c) the influence of residual gases and of the electron beam on nucleation as studied by grazing incidence electron diffraction, mass spectrometry, and light microscopy; and

(1d) the initial growth of metal films on metal and semiconductor single crystal surfaces in UHV as studied by low energy electron diffraction (LEED).

The work falling into category (2) was concerned with the preparation and characterization of clean single crystal surfaces and their interaction with gases. Experimental tools used were LEED and mass-spectrometry; theoretical work on low energy electron scattering supported the LEED experiments.

II. THEORETICAL WORK ON INTERFACIAL ENERGY AND NUCLEATION

This work was stimulated by Harsdorff's experiments [Solid State Comm. 1, 218 (1963); 2, 133 (1964)] which had revealed an oscillatory temperature dependence of the perfection of the orientation of f.c.c. metals on alkali halides. Such an oscillatory dependence is to be expected on the basis of the oscillatory dependence of the interfacial energy upon interface size. This suggested application of the only nucleation theory which includes the size and shape dependence of the interfacial energy [Bauer, Z. Kristallogr. 110, 372, 395 (1958)] to Harsdorff's experiments. While the programming for the IBM 7040 was going on, experiments were reported [Adam, Harsdorff, Z. Naturforsch. 20a, 489 (1965)] which indicated that the oscillatory behavior mentioned above was probably not simply related to the size of the interface but was strongly related to water vapor evolution from alkali halides. The programming was therefore stopped and after we had confirmed the water evolution the theoretical work was postponed until the beginning of our own planned quantitative nucleation work.

III. GROWTH OF f.c.c. METALS ON ALKALI HALIDES IN ULTRAHIGH VACUUM

This work was stimulated by the experiments of Ino, Ogawa and Watanabe [J. Phys. Soc. Japan 19, 881 (1964)] which indicated that the growth of certain f.c.c. metals in UHV on NaCl is quite different from the growth in ordinary vacuum and that the condition of the NaCl surface was quite critical. If meaningful experiments on the influence of the interface on the epitaxial growth are to be done the phenomena observed by Ino et al. have to be understood first. In order to achieve such an understanding experiments were performed which allowed the observation of the film growth in UHV by grazing incidence electron diffraction. Materials investigated were Au on NaCl, KCl, KI, Ag on KCl, and Al on NaCl, i.e. three f.c.c. metals with approximately identical lattice constants. After removal from the UHV system the films were studied by electron microscopy and transmission electron diffraction; in this part of the experiment our work on Au on NaCl overlapped with that of Matthews et al. [Appl. Phys. Letters 5, 166 (1964), 7, 131 (1965); Phil. Mag. 11, 1223 (1965), 12, 1143 (1965)], whose work was done independently of ours. Although our experimental results agree qualitatively with theirs, our interpretation is in important aspects different from theirs. This is mainly due to the larger experimental material available to us, which shows that the growth of f.c.c. metals on clean alkali halide surfaces in UHV is very peculiar for each film-substrate pair, so that from a limited number of experiments no general conclusions can be drawn as was done by Matthews. Some of the differences between Matthews and our interpretation are discussed in Enclosure (1), a full report of our experimental work and its interpretation is in preparation for publication; some of the results obtained before September 1, 1965 have been included in Encl. (1) of the Third Quarterly Progress Report. The results obtained provide a fundamentally new insight into the influence of the interface and the surface of the growing crystals on epitaxial growth and provide the basis for future quantitative work on epitaxial nucleation.

IV. THE INFLUENCE OF RESIDUAL GASES AND OF THE ELECTRON BEAM ON NUCLEATION

The work in this area was concentrated on the nucleation of NaCl on NaCl, but included also observations made in the study of the growth of f.c.c. metals on alkali halides as described in III. Some of the results obtained for NaCl on NaCl have been reported in Encl. (1) of the Second Quarterly Report, indicating a profound influence of certain gases on nucleation. Work to understand the mechanism is still in progress. It involves (1) annealing of NaCl {100} and {110} surfaces in gases and studying their surface structure and the gas evolution from such crystals, (2) experiments on the growth of NaCl cleaved in UHV, and (3) theoretical geometric considerations of the possible interface structures leading to the observed orientations.

The electron beam has also a profound influence on the growth of f.c.c. metals on alkali halides, both on the particle density and particle orientation. For example Au cannot be grown as a single crystal film on NaCl cleaved in UHV, however if the surface is bombarded with electrons immediately before or during evaporation the condensation coefficient is increased considerably and a single crystal film is formed. The beam influence varies considerably with the film-substrate combination and the substrate condition, indicating the complexity of the process. Details will be reported in the publication in preparation mentioned in III.

V. THE INITIAL GROWTH OF METAL FILMS ON METAL SEMICONDUCTOR SINGLE CRYSTALS

The purpose of these investigations was threefold: (1) to check the validity range of a theory of the growth mode of very thin films, i.e. of the problem of two-dimensional versus three-dimensional nucleation [Bauer, Z. Kristallogr. 110, 372 (1958)]; (2) to obtain an understanding of the interface between two crystals; and (3) to collect experience for the formation of complex metal-oxygen surface structure as they are intended to be used later in the study of the relation between electron emission and the structure of surface films. The following systems have been investigated: Ag and Au on a {110} plane of W (see First Quarterly Report), Ag on {111} and {100} planes of Cu (see Second Quarterly Report), Pb on the {110} plane of W and Ag and Au on the {111} plane of Si (see Third Quarterly Report). Some of the major findings are: (1) the existence of one-dimensionally strained monolayers (Pb on W), (2) the formation of ordered interface alloys of metals not miscible in the bulk (Ag on Cu), (3) the strong influence of a chemisorbed gas layer on nucleation (Ag and Au on W), and (4) the considerable differences in the structure of surface films of metals with nearly identical lattice constants and similar electronic structure (Au and Ag on Si). Although we have reported some of the data at conferences we consider their publication as premature until more quantitative experiments are done and the interpretation techniques in low energy electron diffraction are developed better.

VI. CHARACTERIZATION OF SINGLE CRYSTAL SURFACES

Most of the low energy electron diffraction work was concerned with the techniques to produce single crystal surfaces, either clean or with well defined adsorbed layers. Simultaneously efforts were made to develop a quantitative theory of low energy electron diffraction. The experiments dealt with the following surfaces: Ni {111}, {100}, {112}, Cu {100}, {111}, Au {100}, W {110}, Si {111}, NaCl {100}. The structure of the surfaces was studied as function of heat treatment, ion bombardment and in situ reaction with O_2, CH_4, CO and D_2. The gas composition and the desorption products from the surfaces were studied with a quadrupole mass-spectrometer which is in line of sight of the crystals. Some of the results have been reported at a conference (see p. 5), many of them are still waiting for quantitative evaluation. The latter include (1) the various surface structures found on Cu, especially the epitaxy of CuO on Cu, (2) the problem of the nature of the chemisorbed oxygen layer on Ni, i.e. the question whether the layer is mixed (consisting of Ni and O atoms) or unmixed, two- or three-dimensional, (3) the nature of the equilibrium surface structure of the Au {100} and the Si {111} plane as obtained after high temperature annealing, (4) the surface structure on the W {110} plane, (5) the structure and orientation of the reaction products of the W {110} plane with O_2, CO, H_2O, CH_4, and (6) the desorption process of layers formed on the NaCl {100} plane in air. As a result of these investigations the methods to produce well defined surfaces, especially of W, W + O, W + CO which are needed in the second part of the problem, are now well under control.

The main difficulty in the quantitative evaluation of LEED observations is the lack of a proper theory of low energy electron diffraction. A first step to such a theory for crystals is a theory for the scattering of slow electrons by atoms. The theoretical work on this subject has steadily progressed. Because of our interest in crystals consisting of heavy atoms the IBM program has been extended to be applicable to heavy atoms. A highly significant result obtained is the fact that contrary to well established opinion the scattering of slow electrons cannot be described by nonrelativistic quantum mechanics, but requires relativistic quantum mechanics (see Encl. (2)).

PUBLICATIONS

1. E. Bauer: "The Study of the Degree of Order in Adsorption by Electron Diffraction," Colloq. Internat. CNRS No. 152, p. 19 (1965). Note: The manuscript was submitted before the beginning of the grant period; therefore no acknowledgment of NASA support is made, although at the oral presentation new data were reported obtained during the contract period.
2. A. K. Green and E. Bauer: "Gas Induced Orientation of Vapor Deposited NaCl Crystals on NaCl Cleavage Surfaces," J. Appl. Phys., Feb. 1966.
3. E. Bauer, A. K. Green, K. M. Kunz, and H. Poppa: "The formation of Thin Continuous Films from Isolated Nuclei," Akademie der Wissenschaften, Göttingen, in print.
4. E. Bauer, A. K. Green, and K. M. Kunz: "The Growth of Single Crystal Films Free of Impurities," submitted to Appl. Phys. Letters.
5. H. N. Browne and E. Bauer: "The Importance of Relativistic Effects in the Scattering of Slow Electrons," submitted to Phys. Rev. Letters.

INVITED CONFERENCE PAPERS

1. E. Bauer: "The Study of the Degree of Order in Adsorption by Electron Diffraction," Internat. Colloquium on "Adsorption et Croissance Cristalline," Nancy, France, 6-12 June 1965.
2. E. Bauer et al.: "The Formation of Thin Continuous Films from Isolated Nuclei," Internat. Symposium on "Basic Problems in Thin Film Physics," Clausthal-Göttingen, 6-11 September 1965.

The Growth of Single Crystal Films Free of Impurities

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In many physical experiments and technical applications thin films are required which are both single crystalline and free of impurities. Recent experiments[1-8] indicate that the two requirements are frequently incompatible, i.e. that impurities are necessary in order to obtain single crystal films by epitaxy. The experiments[6,8] show that continuous films with good single crystal orientation (formed in the presence of certain impurities) have in the initial stage of formation a much higher particle density than films with poor single crystal orientation (formed under similar conditions in the absence of impurities). On the basis of these observations Matthews[9] has suggested a technique for growing single crystal films of fcc metals on clean alkali halide surfaces in ultrahigh vacuum. This technique which he demonstrated for the growth of Au on NaCl should lead to films free of impurities. Its basic idea is to deposit a very thin layer ($\sim$ 20 Å) of the metal at a very high rate ($\sim$ 1000 Å/sec) immediately after cleaving the crystal at 350°C in ultrahigh vacuum. The high deposition rate is used to obtain a high particle density and consequently early coalescence which is considered by Matthews to be essential for the formation of a single crystal film. The deposition immediately after cleaving ensures that the surface does not get contaminated by the residual gas. It is the purpose of this letter to show that Matthew's suggested procedure is neither sufficient nor necessary for obtaining single crystal films free of impurities; to propose a simpler procedure to achieve this goal and to point out the limitations of both.

Encl. (1)

The procedure used in Matthews technique is not sufficient for two reasons. First, at high evaporation rates Au evolves a large amount of gas which can be incorporated into the growing film. This will lead to epitaxial growth in a similar way as in the experiments done in unbaked vacuum systems.[1-3,5] Because of space limitations a discussion of the arguments for and against this premise will be given elsewhere. The second reason is as follows: Although cleaving during or immediately before evaporation ensures that the surface will not be contaminated from the vacuum, it can be strongly contaminated from the bulk of the crystal. This can be concluded from several observations. Harsdorff[2,10] has found maxima and minima in the perfection of the orientation of fcc metal films grown in a vacuum of about 4.10^{-6} torr on alkali halides as a function of temperature. He assumed that the alkali halide surfaces were covered with several adsorbed water layers and attributed the maxima to the removal of successive water layers. This interpretation seemed to be supported by mass spectrometer observations,[11] which showed H_2O "desorption" peaks at temperatures which could be related to those at which the perfection of the orientation had its maxima. However we have shown[6] that the H_2O peaks are not due to surface layers but result from bulk impurities which reach the surface very rapidly in certain temperature regions by a mechanism to be described elsewhere. H_2O bursts have also been observed upon cleaving of NaCl.[12] Harsdorff's[2,10] observations show that impurities in the bulk influence the film orientation even in a vacuum of the order of 10^{-6} torr. Therefore, in a baked ultrahigh vacuum system where the water partial pressure is very low (e.g. 10^{-10} torr), evaporation during or immediately after cleaving leads, (at least in the temperature regions of strong H_2O evolution), to a stronger impurity influence on the film growth than evaporation onto a surface which had some chance to outgas between cleaving and evaporation.

That the procedure used by Matthews is not necessary follows from the following observation which we have made in many ultrahigh vacuum evaporations of Au: When Au is evaporated simultaneously onto NaCl and KCl cleaved in ultrahigh vacuum, both films have initially the same small number of nuclei (as compared to a surface cleaved in air), with roughly the same orientations. However, while the continuous films of Au on NaCl consist of crystals with their {111} planes parallel to the substrate, those on KCl have a perfect single crystal orientation similar to that in Au films on surfaces cleaved in air. This shows that neither a high density of nuclei nor an air-contaminated surface nor reactive residual gases are necessary in order to obtain a single crystal film. In fact, the film with the lowest number of microtwins or stacking faults and dislocations which we have obtained was grown on a KCl surface cleaved at 4.10^{-8} torr at 180°C and deposited 20 min later at 6.10^{-8} torr at 360°C (see Fig. 1). The transmission diffraction pattern of this film is a perfect Laue pattern with weak Kikuchi bands. This perfection of the single crystal orientation can not be ascribed to H_2O evolution as discussed above for NaCl, because KCl evolves much less H_2O from the bulk than NaCl, and none at all at the deposition temperature. KCl surfaces cleaved in air could be cleaned by heating to 450°C similar to NaCl surfaces. This eliminates the necessity of cleaving KCl in ultrahigh vacuum and simplifies the preparation of single crystal Au films free of impurities.

It should be pointed out that the "impurity free" Au single crystal films may be reasonably free of impurities in the bulk, but there are strong indications that their surfaces are not clean. In situ ultrahigh vacuum reflection electron diffraction results show that beginning with a partially coherent single crystal film of Au a superstructure develops (Fig. 2) which is associated with an impurity-gold compound. This also has been found by low energy electron diffraction,[13,14] and has been attributed to an alkali-gold compound.[13] If this interpretation is correct, the observations indicate that the growth of single crystal films on alkali halides not only depends critically upon the residual gas pressure and composition, the history of the surface and the impurity content in the bulk of the substrate, but is also strongly influenced by interface reactions between film and substrate not known previously.

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Figure 1. Transmission electron micrograph of gold film described in text. Magnification X20,000.

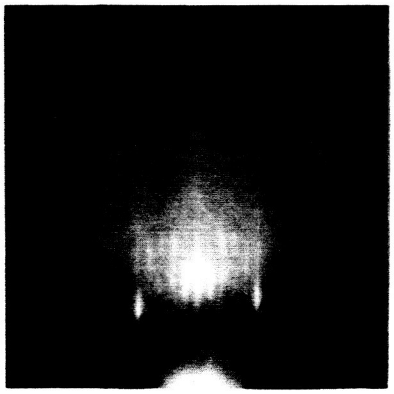

Figure 2. In situ UHV reflection electron diffraction pattern of gold film described in text. ⟨110⟩ Azimuth.

N66-20069

The Importance of Relativistic Effects in the Scattering of Slow Electrons

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In the past it has been generally assumed that the total and differential scattering cross section for slow electrons could be calculated using nonrelativistic quantum mechanics. It is the purpose of this letter to demonstrate that this assumption is erroneous and that relativistic effects play a very important role at low electron energies, at least in the scattering by heavy atoms.

In order to simplify the theoretical treatment we prove our statement in the static central field approximation, i.e. we neglect spin-spin correlation (exchange) and charge-charge correlation (polarization) between the free and the atomic electrons. In this approximation the ℓ^{th} partial wave $F_\ell(r)$ in the partial wave expansion of the scattered wave is obtained from the following equations (in Hartree atomic units):

$$F''_\ell + \left[k^2 + 2V(r) - \frac{\ell(\ell+1)}{r^2}\right] F_\ell = 0 \qquad (1)$$

in the nonrelativistic treatment and

$$F''_\lambda + \left[\frac{1+\gamma}{2} k^2 + 2\gamma\, V(r) - \frac{\ell(\ell+1)}{r^2} + \alpha^2\left(V^2(r) + \frac{\lambda+1}{r}\,\frac{V'(r)}{\gamma+1+\alpha^2 V(r)} + \frac{1}{2}\,\frac{V''(r)}{\gamma+1+\alpha^2 V(r)} - \frac{3}{4}\,\frac{\alpha^2 V'^2(r)}{(\gamma+1+\alpha^2 V(r))^2}\right)\right] F_\lambda = 0 \qquad (2)$$

in the relativistic treatment.

Encl. (2)

Here k^2 is the kinetic energy measured in units of 13.6 eV, $V(r) = \frac{Z(r)}{r}$ is the potential energy of the electron in the field of the atom with $Z(r)$ being the effective nuclear charge, $\gamma = (1-\beta^2)^{-1/2}$ with $\beta = \frac{v}{c}$; $\alpha = \frac{1}{137.037}$ is the Sommerfeld fine structure constant, and λ assumes two values depending on the relative direction of spin $\frac{1}{2}$ and angular momentum ℓ:

$$\lambda^+ = +\ell \text{ if } j = \ell + \frac{1}{2}$$

$$\lambda^- = -(\ell+1) \text{ if } j = \ell - \frac{1}{2} \;.$$

For $\ell = 0$ there is only one equation and $\lambda = 0$.

The differential scattering cross section is obtained from the phase shifts η_ℓ, η_λ^+, η_λ^- of the asymptotic form of the partial waves F_ℓ, F_{λ^+}, F_{λ^-} with respect to the solutions of the Eqs. (1) and (2) with vanishing $V(r)$:

$$I(\theta) = f(\theta)f^*(\theta) \text{ with } f(\theta) = \frac{1}{2ik} \sum_{\ell=0}^{\infty} (2\ell+1)(e^{2i\eta_\ell} - 1)\; P_\ell(\cos\theta) \qquad (3)$$

in the nonrelativistic case and

$$I(\theta) = f(\theta)f^*(\theta) + g(\theta)\, g^*(\theta) \text{ with}$$

$$f(\theta) = \frac{1}{2ik} \sum_{\ell=0}^{\infty} \left[(\ell+1)(e^{2i\eta_\lambda^+} - 1) + \ell(e^{2i\eta_\lambda^-} - 1)\right] P_\ell(\cos\theta) \qquad (4)$$

$$g(\theta) = \frac{1}{2ik} \sum_{\ell=0}^{\infty} \left[e^{2i\eta_\lambda^-} - e^{2i\eta_\lambda^+}\right] P_\ell^1\,(\cos\theta)$$

in the relativistic case.

The total scattering cross section Q is given by $Q = 2\pi\int_0^\pi I(\theta)\sin\theta d\theta$ or by the optical theorem: $Q = \frac{4\pi}{k}\,\mathrm{Im}\, f(0)$. Equation (2) differs from (1) in two aspects: (a) in the first two terms, and (b) in the α^2 term. Aspect (a) represents the relativistic effect proper since these two terms increase with increasing energy. Regarding aspect (b), the terms in the parenthesis are either independent of energy or their moduli decrease with energy. However their contributions are in general small because they are of order α^2 or higher order in α^2. Only near $r = 0$, where $V(r) = \frac{Z(r)}{r}$ has a first order pole, can the terms become significant. This is probably the reason for the general belief that relativistic effects have no influence on $I(\theta)$ and Q at low electron energies as slow electrons do not penetrate very deeply into the atom so that their $I(\theta)$ and Q are largely determined by the outer part of the atom. Although this is true--as indicated by the small amplitude of the partial waves near the nucleus--the potential near the nucleus has nevertheless considerable influence on the phase and amplitude of the partial waves (Fig. 1). For low electron energies ($\gamma \approx 1$) and small r ($Z(r) \approx Z_o$) Eq. (2) simplifies to

$$F''_\lambda + \left[k^2 + 2\frac{Z_o}{r} - \frac{\ell(\ell+1)}{r^2} + \alpha^2 \frac{Z_o^2}{r^2} - \frac{\lambda y + \frac{3}{4} y^2}{r^2}\right] F_\lambda = 0 \qquad (5)$$

with $y = \dfrac{\alpha^2 \frac{Z_o}{r}}{2 + \alpha^2 \frac{Z_o}{r}}$ $(0 \leq y < 1)$.

This equation shows that the influence of the last two terms which distinguish the relativistic from the nonrelativistic case increases with (1) increasing Z_o and (2) the increase of the contributions of the partial waves with small ℓ to the scattering cross section, i.e. with decreasing electron energy.

To determine the magnitude of the influence of the extra terms in the relativistic equations, numerical calculations are necessary. Such calculations have been performed for He, Kr, Cs, and Hg for 2, 20, and 200 eV electrons in order to obtain quantitative information on the energy and Z_o dependence of the difference between nonrelativistic and relativistic scattering cross sections. The total scattering cross sections are shown in Table I, typical differential scattering cross sections in Fig. 2. Most of the calculations were performed with a program written by Hückel and modified by Holtzwarth and Meister[1] which uses a simplified Numerov integration method. The accuracy was checked by varying the integration step size and by comparison with data obtained with another extensively checked program using a Runge-Kutta procedure.[2,9] The atomic potentials used are taken or derived from data given in the references listed in the tables together with the scattering cross sections. In most cases the numerical integration was terminated at $r_{max} \approx 5$, but for Hg at 2 eV the influence of r_{max} on the data was examined and found to be qualitatively insignificant (Table II). For Kr the energy dependence of the contributions of the different partial waves was studied more carefully (Fig. 3).

The results in Table I clearly indicate that the relativistic effects

(1) increase with the nuclear charge Z_o. In He they are hardly noticeable, in Hg they are very large;

(2) decrease with increasing electron energy. At 200 eV they amount only to a few percent in the total scattering cross section Q while at 2 eV they can change Q by an order of magnitude;

(3) exist independent of the type of potential used. The strong variation of the scattering cross sections at low energies with potential which has been noted earlier (see e.g. Ref. 2, Fig. 4) clearly demonstrates the need for better wave functions;

(4) either increase or decrease the total scattering cross section.

A better understanding of the relativistic effects is obtained by studying the partial wave shifts. The numerical data show that in all cases where the relativistic effects are significant, both η_λ^+ and η_λ^- are larger than η_ℓ (see e.g. Fig. 3). This means that the λ-dependent term which represents spin-orbit coupling and which leads to the Mott-polarization of the electrons is smaller than the other terms, so that the relativistic potential is stronger than the nonrelativistic potential. The number of partial waves in which relativistic effects are significant increases with Z_o and k^2: in Kr only η_o and η_1 differ considerably at 2 and 20 eV; in Cs η_o and η_1 at 2 eV, η_o, η_1 and η_2 at 20 eV and 200 eV; in Hg the effects are significant up to η_1, η_2 and η_3 at 2, 20, and 200 eV respectively.

In the light of these results the agreement between the nonrelativistic theory and experiment which has been obtained previously by other authors for the scattering of slow electrons by heavy atoms has to be considered as fortuitous as the agreement obtained for light atoms neglecting spin and charge correlation.[2] This applies not only to the old work, e.g. on Cd and Hg,[10] but also to recent work on Cs.[11-14] We conclude that in order to obtain reliable scattering cross sections of heavy atoms for slow electrons, not only exchange and polarization but also relativistic effects have to be considered.

We would like to thank Dr. Meister for putting Hückel's IBM program at our disposal.

FOOTNOTES

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Table I. Total scattering cross sections of He, Kr, Cs, and Hg for 2, 20, 200 eV electrons

Z_o	Atom	Potential	Case	2 eV	20 eV	200 eV
2	He	Hartree-Fock[3]	rel	76.0	8.20	.752
			nonrel	76.1	8.20	.753
36	Kr	Hartree-Fock[4]	rel	110.	31.7	13.2
			nonrel	108.	29.8	13.3
55	Cs	Hartree-Fock-Slater[5]	rel	228.	65.8	20.7
			nonrel	286.	61.2	21.0
		Thomas-Fermi-Dirac[6]	rel	131.	17.6	15.8
			nonrel	119.	14.0	16.0
80	Hg	Hartree-Fock-Slater[5]	rel	12.8	50.9	21.1
			nonrel	1.55	59.3	20.3
		relativistic Hartree[7]	rel	84.1	15.1	27.2
			nonrel	19.5	23.1	26.7
		Thomas-Fermi-Dirac[6]	rel	99.9	9.82	28.3
			nonrel	393.	13.5	27.9
		Thomas-Fermi[8]	rel	216.	79.9	30.8
			nonrel	328.	68.	31.1

Table II. Influence of r_{max} on the total scattering cross section of Hg for 2 eV electrons

Potential	Case	r_{max} = 4.7	8.2	14.0
Hartree-Fock-Slater[5]	rel	12.8	14.1	14.1
	nonrel	1.55	1.20	1.20
Thomas-Fermi-Dirac[6]	rel	99.9	100.	100.
	nonrel	393.	393.	392.

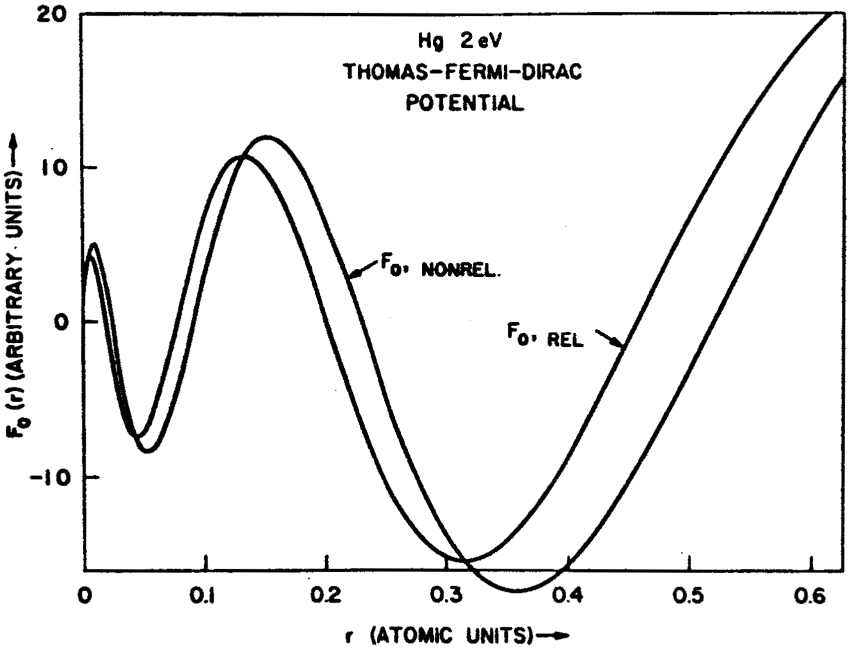

Fig. 1. S-wave for the scattering of 2 eV electrons by Hg. The relativistic and nonrelativistic wave-functions as obtained by solving Eqs. (2) and (1) respectively for $\ell = 0$ are shown only for small r values. At $r_{max} = 8.2$ we obtain $F_{o,\ nonrel} = 76.6$ and $F_{o,\ rel} = 42.9$.

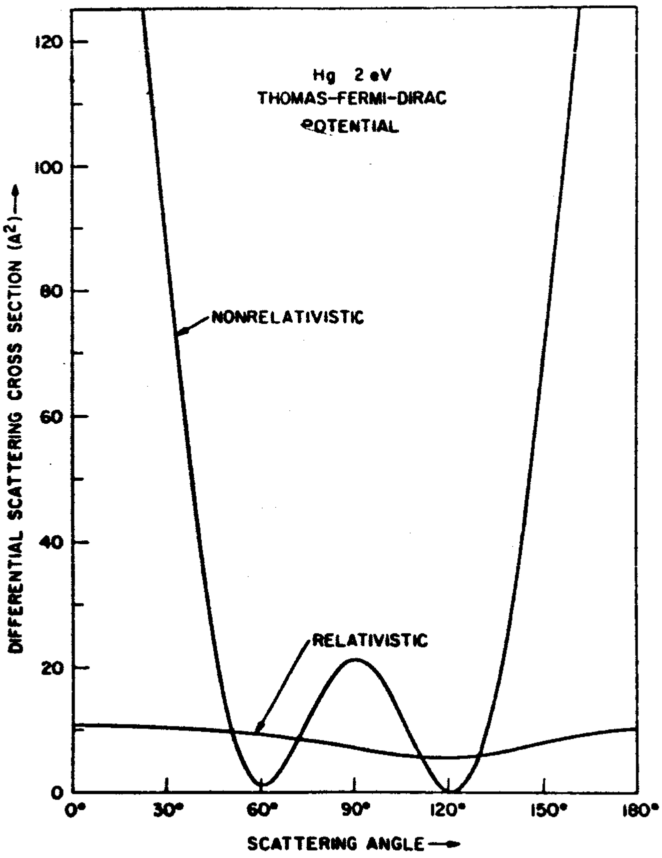

Fig. 2. Differential scattering cross section of Hg for 2 eV electrons.

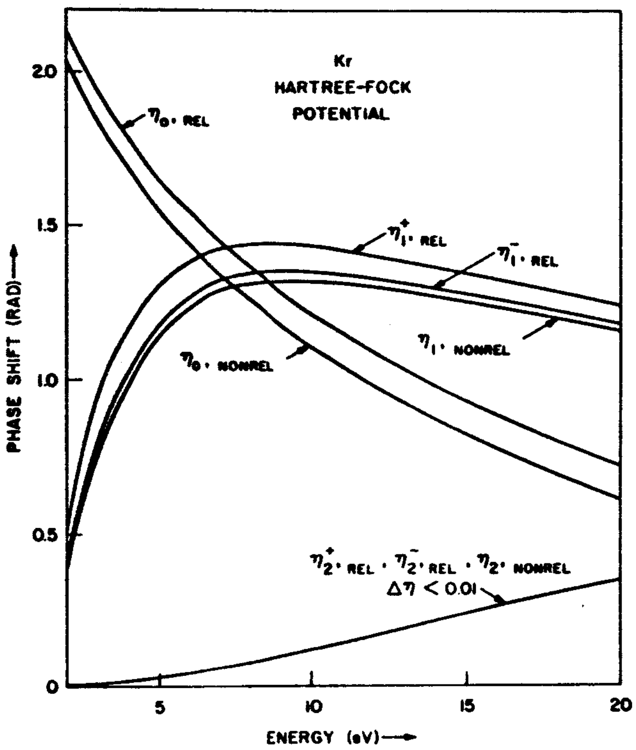

Fig. 3. **Partial wave phase shifts for the scattering of 2 - 20 eV electrons by Kr.**