and are using data taken on it to evaluate the constant terms contained in μ and subsequently using that resulting μ to arrive at a prediction for the BCS region. We have used the value $\mu/(H_{c2} - H) = 0.021$ at $T = 0°K$ for the theoretical lines in 3(a), 3(b), 3(c), and 3(d). Although this is only an extrapolation of low-temperature results, there is surprising agreement between the theoretical and experimental slopes for the gapless region. The experimental slopes in the BCS region lie above the theoretical curve. However, the temperature dependence appears to be similar.

In conclusion we find the predicted BCS and gapless regions in the field dependence of the attenuation of both longitudinal and shear waves. At lower temperatures we find relative agreement between experiment and theory in the shapes of the curves. There is qualitative agreement with the temperature dependence of the slopes in the gapless region. In the BCS region these slopes follow the shape of the temperature-dependent theoretical curves. Clearly more theoretical work is necessary to improve the exact understanding of the regimes as well as the transition from one to the other.

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New Perturbation Theory for Low-Energy Electron-Diffraction Intensities

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Standard perturbation theory applied to the low-energy electron-diffraction problem does not appear to give accurate results even when carried to second order. A new scheme, renormalized forward-scattering perturbation theory, retains the advantage of being fast to execute, but at the same time is very accurate. The new theory is subjected to the stringent test of comparison with exact results for a realistic model of the copper (100) surface.

There are two decisions to be made before embarking on calculations of the diffraction of a monoenergetic, well-collimated beam of electrons incident on a crystal surface. Firstly a model must be postulated for the surface, including the quantities strongly affecting the diffraction process, and omitting quantities that do not strongly affect the process but are possibly difficult to calculate. Secondly, having decided the nature of the environment in which the electron finds itself, a method of solution of the diffraction process must be fixed upon.

In recent years it has become apparent that a model of the surface taking account of the strong elastic scattering by ion cores and of inelastic scattering processes (the ion-core scattering model),[1-3] when combined with an accurate nonperturbative method of calculation, gives good agreement with experiment.[1,3-5] The main concern of this Letter is to suggest a fast, accurate

scheme for solution of the diffraction process. There is a need for such a scheme because the accurate methods employed so far have all been time consuming. For example, my earlier calculation took between 30 and 60 sec per energy at which calculations were made on the ICL Titan computer. Times in the exact methods scale as n^3, n being the number of diffracted beams. Therefore calculations at high energies or for complex surface structures, where n is increased considerably, can involve times being increased to an extent that they are no longer feasible. Even for relatively simple surfaces at low energies an increase in speed would be useful.

Nevertheless, nonperturbative calculations have achieved two essential objectives: They have removed any uncertainty from the details of calculation and thus enabled a fair test to be made of models of the surface. In this way the validity of the ion-core scattering model has been firmly established. Secondly, accurate solutions of this realistic model provide an ideal test of the accuracy of approximate schemes of calculation. Copper has been chosen as a critical testing ground for theories because its low-energy electron-diffraction (LEED) spectrum, in common with those of the transition metals, implies strong multiple scattering. Moreover the exact calculations have already been made for this material.[5]

Perturbative schemes generally have the advantage of being much faster in calculation, and also the times involved scale only as n^2. Thus, the increasing complexity of diffraction patterns is less of a difficulty. One perturbative scheme of calculation is already in existence.[6] In this scheme the scattering is divided into two parts: that within the individual layers of atoms parallel to the surface, and that taking place between layers. The first part is treated exactly; the perturbation theory is developed in terms of scattering by layers. Details can be found in the original paper[6] or in a summary of them, together with details of how the present calculation was performed, in a paper by the present author.[7] The calculations made using this standard perturbation theory for a copper (100) surface under conditions of normal incidence are shown in Fig. 1(a). First- and second-order results are shown together with the exact results for comparison. Agreement is not good even when the series is carried to second order. The same picture is repeated for beams other than the 00, but they are not reproduced here for reasons of space.

Indeed the breakdown of perturbation theory in LEED for the transition metals was predicted in an earlier paper.[1] A necessary condition for convergence is that inelastic processes should dominate the scattering, a condition that can be understood by noting that inelastic scattering events remove electrons from the diffraction process completely at a rate determined by the inelastic scattering matrix element V_i. The rate at which electrons are elastically scattered

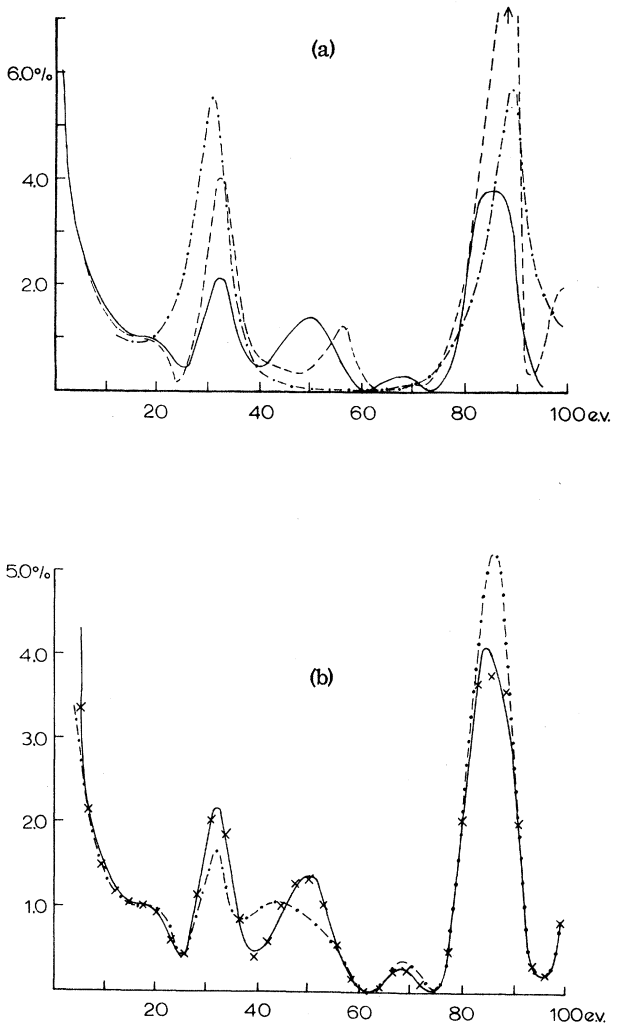

FIG. 1. (a) Comparison of first-order (dot-dashed line) and second-order (dashed line) perturbation theory calculations with the exact results (solid line) for the 00 beam incident normal to a copper (100) surface. (b) Comparison of RFS perturbation theory calculations for first order (dot-dashed line) and third order (crosses) with the exact results (solid line) for the 00 beam incident normal to a copper (100) surface.

is determined by the elastic scattering matrix elements V_e. After an elastic scattering event, the electron remains to be scattered again. If the elastic scattering is taking place more rapidly than absorption by inelastic scattering, i.e., if

$$V_e > V_i, \tag{1}$$

many elastic scatterings occur, on the average, before the electron is removed by an inelastic scattering and the perturbation series has to be carried to many orders. Conversely, the condition

$$V_e \ll V_i \tag{2}$$

says that only one or two elastic scatterings take place, and only one or two orders of the perturbation series are required to describe the situation accurately.

If a successful perturbation theory is to be found, the rule must be that all scattering with matrix elements larger than V_i must be treated exactly. In the earlier paper[1] the observation was made that not all elastic scattering matrix elements are large. Only those for forward scattering are big; those for back-scattering are small and suitable for a perturbative treatment.

Fortunately it proves to be easy to solve for the forward scattering exactly. By making the standard approximation that ion-core scattering is confined to spherically symmetric, nonoverlapping muffin tins about each ionic site, and that in between muffin tins the electron experiences a uniform potential V_0 which includes an imaginary component to take account of absorptive processes, the wave function between the hth and $(h-1)$th layers of muffin tins can be written as a sum over forward and backward traveling plane waves:

$$\sum_{\vec{g}}\{U_{h\vec{g}}{}^{+}\exp[i\vec{K}_{\vec{g}}{}^{+}\cdot(\vec{r}-h\vec{a})]+U_{h\vec{g}}{}^{-}\exp[i\vec{K}_{\vec{g}}{}^{-}\cdot(\vec{r}-h\vec{a})]\}, \tag{3}$$

$$\vec{K}_{\vec{g}}{}^{\pm}=(\pm(2E-2V_0-K_{g_y}{}^{2}-K_{g_z}{}^{2})^{1/2},K_{0y}+g_y,K_{0z}+g_z), \tag{4}$$

where $\vec{a}$ is the displacement of the hth layer relative to the $(h-1)$th layer, $\vec{g}$ is a reciprocal-lattice vector of the surface, E is the energy of the wave incident on the surface, and K_{0y} and K_{0z} are components of the wave vector of the incident wave parallel to the surface; $U_0{}^{+}$ is the amplitude of the incident wave and $U_0{}^{-}$ that of the reflected wave.

In the absence of scattering, the forward-traveling waves between the hth and $(h-1)$th layers propagate to between the jth and $(j-1)$th layers unimpeded:

$$\sum_{\vec{g}}U_{j\vec{g}}{}^{+}\exp[i\vec{K}_{\vec{g}}{}^{+}\cdot(\vec{r}-j\vec{a})]=\sum_{\vec{g}}\sum_{\vec{g}'}P_{\vec{g}\vec{g}'}{}^{+}(j-h)U_{h\vec{g}}{}^{+}\exp[i\vec{K}_{\vec{g}}{}^{+}\cdot(\vec{r}-j\vec{a})], \tag{5}$$

where

$$P_{\vec{g}\vec{g}'}{}^{+}(j-h)=\exp[i\vec{K}_{\vec{g}}{}^{+}\cdot(j-h)\vec{a}]\delta_{\vec{g}\vec{g}'}; \tag{6}$$

P^+ is called the propagator. When the forward scattering is strong, there are many other contributions to $U_j{}^{+}$ involving scattering at intermediate layers. A typical contribution might involve propagation to the kth layer via $P^+(k-h)$, forward scattering there represented by M^+, further propagation to the lth layer via $P^+(l-k)$ followed by another forward scattering event involving M^+, and finally propagation to the jth layer via $P^+(j-l)$. All these contributions give

$$P_{\mathrm{RFS}}{}^{+}(j-h)=P^+(j-h)+\sum_{h\le k<j}P^+(j-k)M^+P^+(k-h)+\sum_{h\le k<l<j}P^+(j-1)M^+P^+(1-k)M^+P^+(k-h)+\cdots. \tag{7}$$

By bearing in mind that

$$P^+(j-h)=[P^+(1)]^{j-h}, \tag{8}$$

this series can be summed to give

$$P_{\mathrm{RFS}}{}^{+}(j-h)=[P^+(1)(1+M^+)]^{j-h}; \tag{9}$$

$P_{\mathrm{RFS}}{}^{+}$ describes propagation from j to h with all possible forward scattering processes included. It will be referred to as the renormalized forward-scattering (RFS) propagator.

Now a new perturbation series in back scattering by layers, represented by M^-, can be developed. The back scattering being small relative to the absorption, there is every reason to believe that a highly convergent series will result. For example, to first order, contributions to the reflected amplitudes $U_0{}^{-}$ come from RFS propagation to the hth layer, $P_{\mathrm{RFS}}{}^{+}(h)$, back reflection at the hth layer, M^-, followed by

renormalized propagation out of the crystal, $P_{RFS}^{-}(h)$. P_{RFS}^{-} has a definition analogous to that of P_{RFS}^{+}:

$$P_{RFS}^{-}(j-h) = [(1+M^{+})P^{-}(1)]^{j-h}. \quad (10)$$

The first-order expression is

$$U_0^{-(1)} = \sum_h P_{RFS}^{-}(h) M^{-} P_{RFS}^{+}(h) U_0^{+}. \quad (11)$$

The next order to contribute to U_0^{-} is third order, only odd numbers of back scattering contributing.

First- and third-order contributions are shown in Fig. 1(b) and compared with the exact results. Even first-order theory gives quite accurate results and after the next contribution has been added, the result is so accurate that it is almost indistinguishable from the original. The new scheme is also very fast. Times taken, once the transmission and reflection coefficients of the individual layers are known, including thirteen beams in the calculation, are 3 sec per point for third-order RFS perturbation theory scaling to about $1\frac{1}{2}$ sec on an IBM machine because of the lower single-precision accuracy. It is hoped that the new RFS perturbation theory will greatly facilitate the application of LEED to the analysis of surface structures.

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Influence of Radiation Damage on Hyperfine-Interaction Measurements after Implantation in Metals

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We report electron microscopy experiments showing that the spatial distribution of damage produced in metals by implanted ions is generally quite different from that of the ions themselves. We discuss how this affects hyperfine-interaction measurements.

Ion implantation is a very powerful method for avoiding metallurgical difficulties in sample preparation. It has been widely used in radioactive hyperfine-interaction (hfi) measurements—i.e., Mössbauer effect, perturbed angular correlations, and nuclear orientation—for which the total number of impurity atoms need not be very large (typically less than 10^{15}).[1,2] However, size differences distort the lattice around the impurity, and radiation damage due to the implantation process produces defects which behave like impurities and interact with implanted ions. It has long been expected that this affects the final position of the foreign atoms and the stability of the alloys formed by this method. Recent experiments[2,3] have shown that this is indeed the case in many instances, where part of the radioactive nuclei cannot be accounted for in nuclear orientation and integral–angular-correlation experiments, the oscillation amplitude is considerably reduced in differential angular correlations, or different sites appear in Mössbauer spectra.

It is often stated[2] that the impurity ion comes to rest in a vacancy-rich area from which most interstitial host atoms created by previous primaries have been projected forward at a rather large distance. Since these interstitials are very mobile at room temperature in most metals, and because *large* impurities tend to occupy lattice sites by replacement collisions, substitutional sites are favored for these impurities. Moreover, in this particular case, the elastic strain of the lattice may be reduced by the attraction of a vacancy to the foreign atom; the important