[3] The relevant formula reads

$$T = s + (-1)^m (s^2 - 1)^{1/2}$$

where

$$s \equiv -\sin(K_0 d + \varphi)/|\varrho|\,,$$

K_0 being the projection of the primary-wave propagation vector on the inward surface normal, d the atom-layer spacing, φ the phase of the amplitude transmission coefficient of a single atom layer and ϱ the amplitude reflection coefficient of an atom layer. The integer m determined by

$$m\,\pi \leqq K_0 d + \varphi + \arcsin|\varrho| \leqq (m+1)\,\pi\,.$$

Formulas like the above appear in many places; see e.g. E. G. McRae, Surface Sci. **25**, 491 [1971], Appendix.

[4] C. M. K. Watts, J. Phys. C **1**, 1237 [1968]. The identity referred to appears on p. 1241 of Watt's paper.

[5] P. J. Jennings and E. G. McRae, Surface Sci. **23**, 363 [1970].

[6] I. S. Gradshteyn and I. M. Ryzhik, Table of Integrals Series and Products, 4th Ed., Academic Press, New York, 1965. Integral number 3.644.4.

[7] J. C. Slater, Phys. Rev. **51**, 840 [1937].

The Optical Potential in Electron Diffraction

A. Howie and R. M. Stern [*]

Cavendish Laboratory, Cambridge, England

(Z. Naturforsch. **27 a**, 382—389 [1972]; received 4 December 1971)

Dedicated to Prof. Dr. K. Molière *on the occasion of his 60-th birthday*

Expressions are derived for the optical potential and related mean free path as a function of energy in the range 20 eV to 100 keV for electrons and estimates are made of the contributions from the electronic excitations, thermal diffuse scattering and disorder scattering in Al, Cu and Au.

Introduction

The significance of the limited penetration of Bloch waves in real crystals was appreciated and the consequences for the angular position and width of the reflected intensity considered comparatively early in the development of electron diffraction theory [1–3]. The concept of a complex potential $(V = \sum_g V_g{}^r + i\,V_g{}^i)$, already used in the quantum theory of scattering by Dirac [4], was introduced by Slater [5] and independently by Molière [6] as a convenient phenomenological device for handling such absorption effects in electron diffraction. At this stage, when the theoretical and experimental emphasis was on reflection diffraction at high energies, attention was focussed on the background absorption effect associated with a mean free path (Λ = intensity attenuation distance) related to $V_0{}^i$, the average value of the imaginary part of the optical potential: $\Lambda = \hbar\,v/2\,V_0{}^i$, where v is the electron velocity [**].

Some fifteen years later the development of transmission electron diffraction and electron microscopy techniques allowed more direct observations of the effect of absorption on the fine structure of diffraction spots [7], the attenuation of Pendellösung fringes [8, 9], and the form of extinction contours [9] and convergent beam patterns [10]. In addition to the background absorption effects associated with $V_0{}^i$. anomalous absorption effects associated with the Fourier components $V_g{}^i$ of the imaginary part of the optical potential became apparent. The variation in the attenuation of different Bloch waves is determined by the form of the periodic intensity distribution of the particular Bloch wave field: the proper development of any theory of electron diffraction therefore requires knowledge of the details of the appropriate optical potential.

The basic theory of the complex potential was given by Yoshioka [11], who using the Thomas-Fermi model, specifically considered the contributions to the real and imaginary part of the optical potential by electronic excitations. In his notation

$$C^r_{00} = V^r_0\,,\quad C^i_{00} = V^i_0\,,\quad C^r_{0g} = V^r_g\,,\quad C^i_{0g} = V^i_g\,.$$

Yoshioka's theory was further developed for electronic excitations [12] and for thermal diffuse scattering [13, 14] by a number of authors. In addition, Hall

---

Reprint requests to Dr. A. Howie, Cavendish Laboratory, Department of Physics, University of Cambridge, *Cambridge*, England.

[*] On leave from Department of Physics, Polytechnic Institute of Brooklyn.

[**] At nonrelativistic energies, $\Lambda = 2\,E^{1/2}/V_0{}^i$ with E and $V_0{}^i$ in eV, Λ in Å.

and Hirsch[15] developed a somewhat more direct method of calculating the imaginary parts of the complex potential V_0^{i} and V_g^{i} for the case of thermal diffuse scattering. At the present time there is general agreement that nearly all the contribution to V_g^{i} and a large part of V_0^{i} arises, in the case of fast electron scattering ($>10^4$ eV), from thermal diffuse scattering. There is a contribution to V_0^{i} (relatively more important in low atomic number materials) from electronic excitation. A useful review of the subject up to this point, given by Kambe and Molière, contains a helpful and more complete list of references[16].

In recent years there has been considerable renewed interest in the case of reflection electron diffraction in the energy range 20 eV – 1000 eV (LEED) where the approximations usually made in high energy electron diffraction are no longer valid.

It has long been recognized[17] that the observed widths (in terms of energy or angle) of apparent Bragg reflections are at certain energies an order of magnitude larger than that predicted by elastic scattering theory. This fact is usually interpreted as resulting from the heavy damping of the Bloch waves, which results in values of V_0^{i} which are particularly large in the energy range of 50 – 1000 eV. However, the complexities of the elastic scattering problem in these experiments and the fact that the measurements are limited to the position, height and width of reflected intensities make it impossible to deduce unique optical potential data from the observations[18]. Nevertheless the electron mean free path is introduced as a fitting parameter in most modern dynamical, inelastic LEED theories[19–21].

Since the optical potential is common to the formalism of electron scattering at all energies and geometries, it appears as a possible unifying and simplyfying concept second in importance only to the Bloch theory. In the hope of establishing some guidelines as to the usefulness of various models for constructing the optical potential, we present in the following sections some of the existing theoretical data supplemented with additional elementary calculations. It is intended to indicate the general trend of the magnitude of the contributions of several different physical mechanisms leading to absorption, as a function of electron energy and scattering crystal type. Although the exact picture of the way in which these quantities depend on the magnitude of the diffraction parameters is not clear, some definite conclusions can be made regarding the relative merits of the choice of experimental variables, and attention is also drawn to those problems which require additional experimental and theoretical effort.

Electronic Excitations

Electronic excitations contribute to an effective absorption in electron diffraction experiments, because energy-loss electrons are excluded from the detector by energy filtering (as is typical in most LEED experiments), or when energy filtering is not employed (as in most electron microscope work), all electrons scattered outside the objective aperture angle are excluded by geometry. Inelastically scattered electrons passing through the aperture generally give contrast effects very similar to those of elastically scattered electrons[22] and are considered part of the elastic wavefield ***. Values of V_0^{i} and V_g^{i} for the electron microscope case have been obtained by Whelan[12] using a single electron matrix element calculation, with Hartree-Fock atomic wave functions, and considering all processes with momentum transfer exceeding a minimum value of $q_{\mathrm{m}} = 0.5$ Å^{-1} corresponding to a typical objective aperture. In agreement with the results of Yoshioka[11], the magnitudes of V_g^{i} are found to be extremely small but there can be an appreciable contribution to V_0^{i} from the outer valence electrons. The effect of inner core electrons is normally negligible. Table 1 (column 2) contains a list of values for V_0^{i} at 100 keV for Al, Cu and Au computed after Whelan[12] from a formula due to Lenz[23], and shown for several different values of q_{m}. The

Table 1. Dependence of the total electronic contribution ($0 \leqq q \leqq \infty$) to V_0^{i}, on the value of q_{m}.

		V_0^{i} $q < q_{\mathrm{m}}$	V_0^{i} $q > q_{\mathrm{m}}$	V_0^{i} total
Aluminum	$q_{\mathrm{m}} = 0.5$ Å^{-1}	−.27 eV	−.57 eV	−.84 eV
	$q_{\mathrm{m}} = 1.35$ Å^{-1}	−.36 eV	−.23 eV	−.59 eV
Copper	$q_{\mathrm{m}} = 0.5$ Å^{-1}	−.32 eV	−.97 eV	−1.29 eV
	$q_{\mathrm{m}} = 1.50$ Å^{-1}	−.45 eV	−.44 eV	−.99 eV
Gold	$q_{\mathrm{m}} = 0.5$ Å^{-1}	−.40 eV	−1.37 eV	−1.77 eV
	$q_{\mathrm{m}} = 1.33$ Å^{-1}	−.56 eV	−.76 eV	−1.32 eV

*** Those processes which contribue to the effective absorption are therefore only those which scatter electrons out of the elastic wavefield, as defined by the limit of resolution (either in angle or energy) of the detection system.

effect of collective excitations of the valence electrons, which is certainly important at small values of q, is ignored by Whelan who uses the tight binding approximation.

An alternative approach which is free from this defect may be based on the dielectric constant formalism using the general relation

$$\frac{1}{\Lambda}=\frac{2\,e^2}{\pi\,\hbar\,v^2}\int_0^\infty\int_0^\infty \operatorname{Im}\left(-\frac{1}{\varepsilon(\boldsymbol{q},\omega)}\right)\frac{q\,\mathrm{d}q\,\mathrm{d}\omega}{q^2+q_0^2} \tag{1}$$

where v is the electron velocity, and q_0 the minimum possible momentum transfer for an energy loss $\hbar\,\omega$ and is related to the incident electron wavevector in the crystal k_0 by;

$$\frac{\hbar^2}{2\,m}\left(k_0{}^2-(k_0-q_0)^2\right)=\hbar\,\omega\,. \tag{2}$$

The most complete calculations of this type have been made [24] for the free electron case where the dielectric constant can be calculated for all values of q and ω in the random phase approximation (R.P.A.). Values of $V_0{}^{\mathrm{r}}=E(\boldsymbol{k})$, and $V_0{}^{\mathrm{i}}=\Gamma(\boldsymbol{k})$, the real and imaginary parts of the optical potential respectively, from a recent calculation of LUNDQVIST [25], are shown as a function of incident electron energy E_0 in Figs. 1 and 2 for the case of aluminum. Such calculations are extremely valuable, but they cannot easily be extended beyond the free electron approximation: the presence of the lattice potential modifies the dispersion relations for the external electron (and hence, for example [26] q_0) and is expected to alter the excitation spectrum for both single electron and collective excitations. In particular, at values of q exceeding some critical value q_{c}, the R.P.A. must break down because of the effects of Bragg reflection: In an f.c.c. structure with lattice parameter a_0, q_{c} is given by:

$$q_{\mathrm{c}}=0.5\;g_{\mathrm{III}}=\pi\sqrt{3}/a_0\,. \tag{3}$$

These complications should not be too serious in aluminum which exhibits a free electron plasma loss and in which contributions to $V_0{}^{\mathrm{i}}$ from values of q in excess of the limit given by Eq. (3) appear to be very small. In metals such as copper and gold, the validity of the free electron model is more questionable however, and to obtain results in these cases we have preferred to use Eq. (2) with values for $\varepsilon(\boldsymbol{q},\omega)$ based on electron scattering and optical data [27]. At present these data are confined to $q=0$ so that the actual q-dependence of ε is ignored. We therefore obtain from Eq. (3), by restricting the upper limit of the integration to be q_{c}, an expression from which the mean free path can be simply determined:

$$\frac{1}{\Lambda}=\frac{2\,e^2}{\pi\,\hbar\,v^2}\int_0^\infty \operatorname{Im}\left(-\frac{1}{\varepsilon(0,\omega)}\right)\ln\left(\frac{q_{\mathrm{c}}}{q_0}\right)\mathrm{d}\omega\,. \tag{4}$$

Values of Λ as a function of incident electron energy calculated in this way using the value of q_{c}, defined by Eq. (3), are shown for Al, Cu and Au in Figs. 3, 4, and 5. These values of $V_0{}^{\mathrm{i}}$ for Al are compared with LUNDQVIST'S [25] data in Figure 1. Considering that these calculations neglect plasmon dispersion (the origin of the discrepancy between the two results at low energies) as well as single electron excitations at values of q larger than q_{c} and the rather arbitrary choice of the magnitude of q_{c}, the close agreement with the more accurate calculation at high energies is undoubtedly fortuitous. An expression for $V_0{}^{\mathrm{r}}$ for the free electron case has been derived by ICHIKAWA and OHTSUKI [28] under similar assumptions:

$$V_0{}^{\mathrm{r}}=-\hbar\,\omega_{\mathrm{P}}\,\lambda/8\,a_{\mathrm{H}}\,. \tag{5}$$

Examination of Fig. 2 shows that their results are in quite close agreement with those of Lundqvist at high energies. It is of interest to note that the increase in the magnitude of the inner potential V_0 due to $V_0{}^{\mathrm{r}}$ would be barely detectable at high energies with the present accuracy of measurement. Optical potential calculations have also been made by HIRABAYASHI [29], although there appears to be a significant discrepancy between his values and the data shown here.

To determine the total contribution to the effective absorption by both collective excitations and single electron scattering one can redefine our cutoff value from q_{c} to q_{m}, and then add the results of our calculations for $q<q_{\mathrm{m}}$ to those of Whelan for $q>q_{\mathrm{m}}$. The total values of $V_0{}^{\mathrm{i}}$ so obtained (see Table 1, column 3) exhibit a considerable dependence on the value chosen for q_{m}. The tight binding method evidently gives much larger contributions to $V_0{}^{\mathrm{i}}$ for $q\sim 1$ Å^{-1} than does our method. In the case of Al where the total greatly exceeds the Lundqvist value, it seems particularly clear that the tight binding method must be unreliable.

Our use of empirical values of the dielectric constant ε (themselves mainly determined from elec-

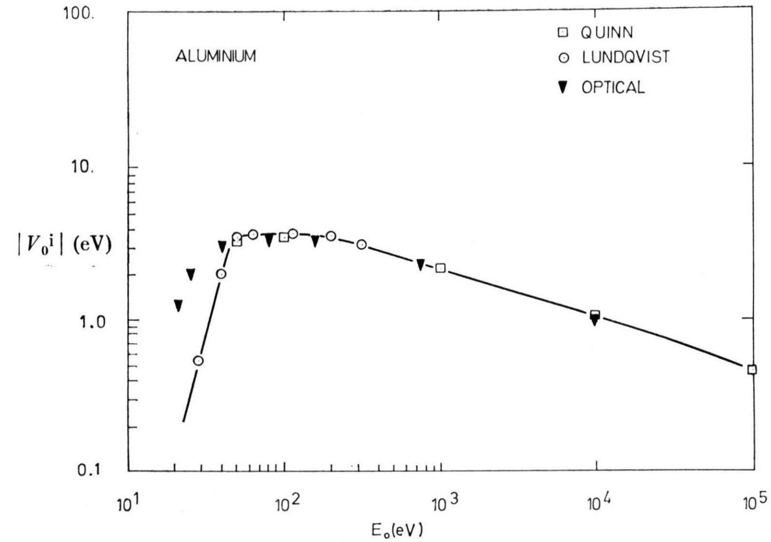

Fig. 1. $V_0{}^{\mathrm{i}}$ vs. electron energy (E_0) in the crystal due to electronic excitations for Al. The agreement between the high energy contribution calculated on the basis of optical data, and from the models of QUINN[24] and LUNDQVIST[25] is probably fortuitous.

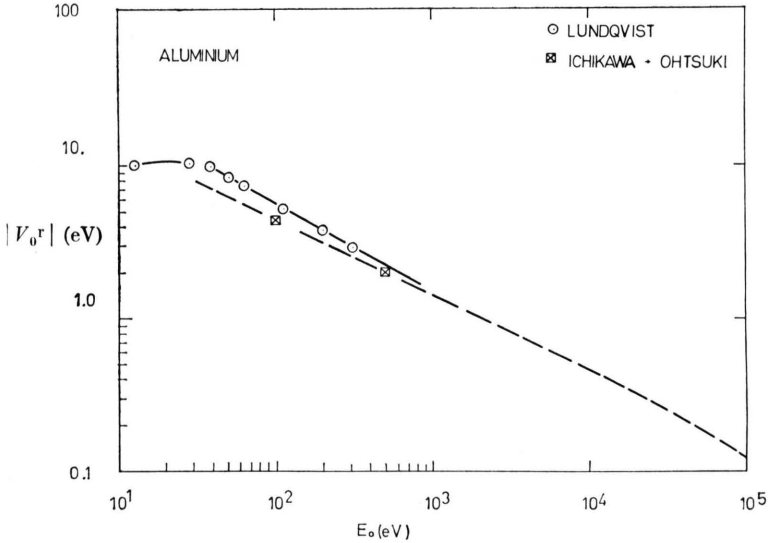

Fig. 2. $V_0{}^{\mathrm{r}}$ vs. electron energy (E_0) for Al, due to electronic excitations, calculated from the models of LUNDQVIST[25] and ICHIKAWA and OHTSUKI[28].

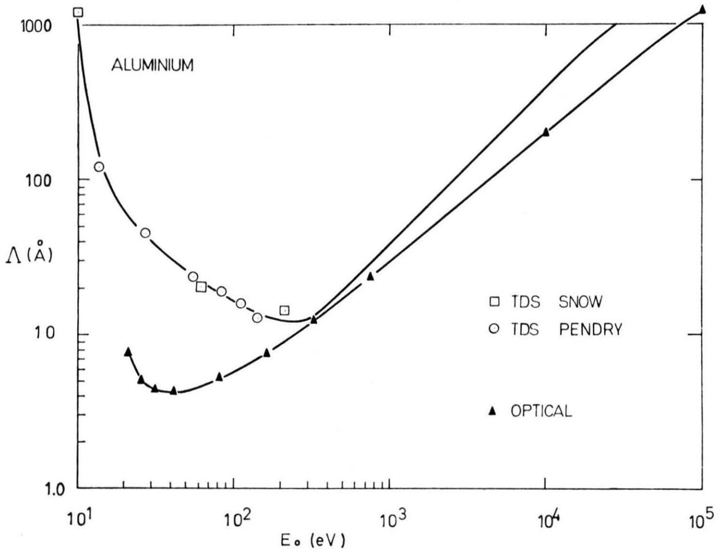

Fig. 3. Electron mean free path Λ as a function of electron energy E_0 for thermal diffuse scattering (TDS) using the phase shift data of SNOW[33] and PENDRY[34], compared to that due to electronic excitations determined from optical data, for Al.

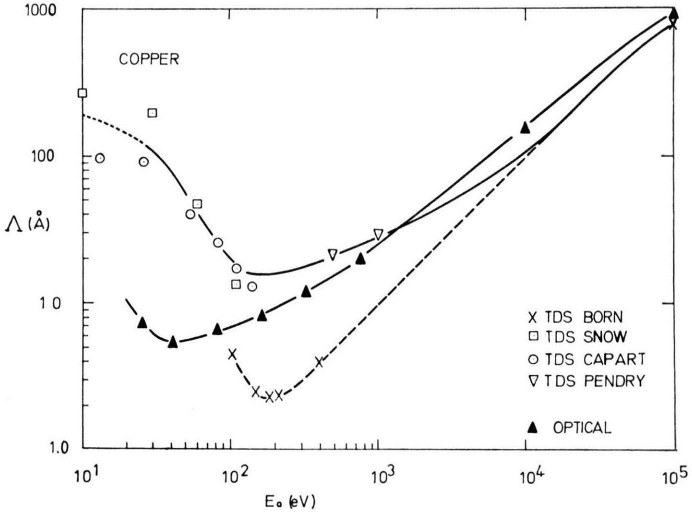

Fig. 4. Electron mean free path Λ as a function of electron energy E_0 for thermal diffuse scattering (TDS) using the phase shift data of SNOW[33], CAPART[35] and PENDRY[34], compared to that due to electronic excitations determined from optical data, for Cu. The TDS mean free path using the Born approximation is also shown for comparison.

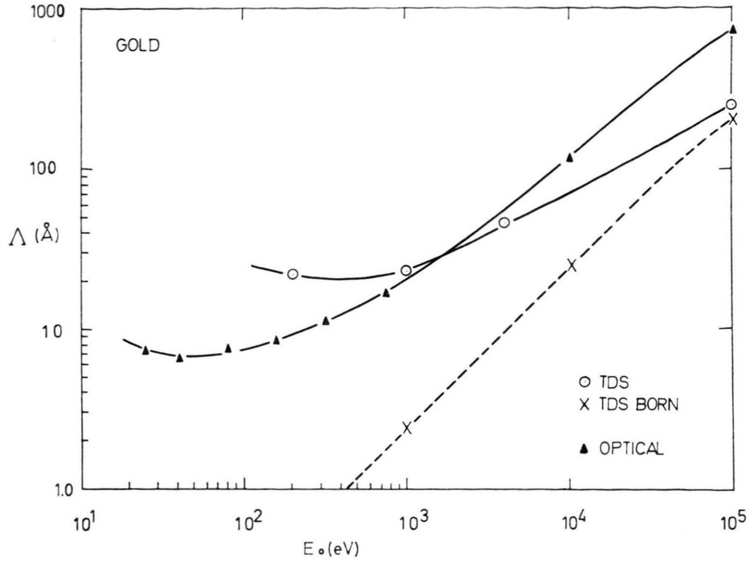

Fig. 5. Electron mean free path Λ as a function of electron energy E_0 for thermal diffuse scattering, based on the Hg data of KESSLER and LINDNER [36]- compared to that due to electronic excitations determined from optical data, for Au.

tron scattering measurements) to calculate $V_0{}^{\mathrm{i}}$ is of course purely a device to connect values of Λ measured at one electron energy to those expected at other energies. It would certainly be useful for this purpose to have good data for $\varepsilon(q, \omega)$ for non-zero values of q, and there seems to be no reason why this cannot be easily obtained, in particular for a variety of materials. In the case of Xenon for example, the application of Eq. (5) yields values of $V_0{}^{\mathrm{i}} < 1.5$ eV which are significantly smaller than the values of ~ 3.5 eV indicated by the LEED experiments [30]. The relatively large lattice parameter in this case leads to a rather small value of q_c for the R.P.A. limit [Eq. (3)] however, and the breakdown of the R.P.A. may be important. It is also of interest to note that the dielectric constant approach of Eq. (2) can be generalised to include the effects of retardation and Cerenkov radiation for high energy electrons [27].

Thermal Diffuse Scattering

An electron which has undergone thermal diffuse scattering cannot normally be excluded by conventional energy filtering methods, and will contribute to the background intensity between the Bragg spots in the diffraction pattern. Frequently however these spots are selected by means of an aperture (either in the microscope, or in the Faraday cage in LEED measurements) so that diffusely scattered electrons are excluded (by momentum selection) and hence contribute to the effective absorption.

Values of the mean free path for thermal diffuse scattering are most conveniently calculated in terms of the atomic scattering amplitudes $f(S)$ ($S = 2 \sin \Theta/\lambda$) using the formula of HALL and HIRSCH [15]:

$$\frac{1}{\Lambda} = \frac{2\,V_0{}^{\mathrm{i}}}{\hbar\, v} \qquad (6)$$

$$= \frac{8\,\pi^3\,\hbar^2}{\Omega\, m^2\, v^2} \int_0^{S_{\mathrm{m}}} |f(S)|^2\,(1 - \exp\{-2\,M_{\mathrm{s}}\})\,S\,\mathrm{d}S$$

where Ω is the atomic volume, $S_{\mathrm{m}} = 2/\lambda$, and the other symbols have their conventional meaning. For room temperature calculations in Al, Cu and Au the appropriate values of α in the Debye-Waller factor $\exp\{-2\,M_{\mathrm{s}}\} = \exp\{-\alpha\,S^2\}$ are:

$\alpha_{\mathrm{Al}} = 0.41$ Å^2, $\alpha_{\mathrm{Cu}} = 0.285$ Å^2, $\alpha_{\mathrm{Au}} = 0.30$ Å^2.
At high electron energies, where the Born approximation is valid and the upper limit of the integral in Eq. (6) is effectively infinite, the value of the integral is proportional to $(m/m_0)^2$ and Λ is proportional to $m_0\,v^2$. In this range our results obtained using the scattering amplitudes of DOYLE and TURNER [31], agree with those of HUMPHREYS and HIRSCH [32]. At lower energies, exchange effects together with the breakdown of the Born approximation can be serious, and the accurate values of $f(S)$ which are required are best obtained from phase

shift calculations:

$$f(S) = \frac{\lambda}{4\pi i} \sum_{l=0}^{\infty} (2l+1) [\exp\{2i\delta_l\} - 1] \cdot P_l(\cos 2\Theta) \qquad (7)$$

where 2Θ is the scattering angle.

At very low energies (less than 100 eV) where $4\alpha/\lambda^2 \ll 1$, the exponential can be expanded and the integration in Eq. (6) carried out analytically to first order in α. This leads to a simple expression for the mean free path in terms of the phase shifts:

$$\frac{1}{\Lambda} - \frac{2\alpha}{\pi\Omega} \sum_{l=0}^{\infty} (l+1) \sin^2(\delta_{l+1} - \delta_l) . \qquad (8)$$

In the intermediate energy range (100 – 10,000 eV) the integral must be evaluated numerically. In Al we have used the phase shift data of SNOW [33] and PENDRY [34] and in Cu that of SNOW [33] and CAPART [35]. Pendry has also kindly supplied us with his unpublished data for Cu in the range 200 – 2000 eV calculated with a Hartree-Fock potential with allowance for exchange effects. Values of $|f(S)|^2$ for H_g in the range of 200 – 4000 eV are given by KESSLER and LINDNER [36] and we have used these data for the Au calculation: since it appears that the two atoms differ only very slightly for this purpose [37].

The values of Λ for Al, Cu and Au are plotted as a function of internal energy E_0 in Figs. 3, 4, and 5, for comparison with the electronic excitation contribution. Clearly the thermal diffuse scattering effect is of little importance in LEED experiments below 100 eV, but it can be quite significant at all energies above 200 eV. The effect of the breakdown of the Born approximation even at relatively high electron energies can be seen in Figures 4 and 5. Examination of the Al potential of BOUDREAUX and HOFFSTEIN [38] indicates that the Born approximation is not seriously in error for this material above 200 eV.

In their thermal diffuse scattering theory, HALL and HIRSCH [15] also give an expression for $V_g{}^i$ in terms of a double integral involving $f(S)$ and $f(|\boldsymbol{S} - \boldsymbol{g}|)$ rather than $|f(S)|^2$. At 100 keV, $V_g{}^i$ can be comparable in magnitude with $V_0{}^i$ and it would clearly be of interest to calculate values of $V_g{}^i$ at lower energies, where the effect of anomalous absorption may be of interest as well ****. Such calculations have however not yet been carried out.

Thermal diffuse scattering also makes a negative contribution to $V_0{}^r$ which has been calculated by ICHIKAWA and OHTSUKI [28]. Their values of several eV obtained at low energies (<100 eV) must be too large by a considerable amount because of their use of the Born approximation. The magnitude of this contribution to $V_0{}^r$ is about .02 eV at 100 keV in Al, and it seems unlikely that this contribution will numerically exceed 1 eV at any energy.

Disorder Scattering

We have so far only considered the contributions to the effective absorption in a perfect lattice. The random potential in a disordered alloy also gives rise to a diffuse scattering in the diffraction pattern and hence makes a contribution to the optical potential. This effect has been considered by HALL et al. [40] for the case of impurities in Si taking account of the effect of both substitutional and interstitial impurities, and also of the surrounding atomic displacements due to size effects. The scattering depends on the scattering amplitude $\Delta f(\boldsymbol{S})$ of the difference between the potential near each impurity centre and the average lattice potential. For a concentration n of centres each at a point $\boldsymbol{r}_i$ in the unit cell, one obtains for the disorder scattering contribution to the mean free path:

$$\frac{1}{\Lambda} = \mu_0 = \frac{2V_0{}^i}{\hbar v} = \frac{4\pi^2\hbar^2 n}{\Omega m^2 v^2} \int_0^{S_m} \int_0^{2\pi} |\Delta f(\boldsymbol{S})|^2 S \, dS \, d\varphi , \qquad (9)$$

$$\Delta\mu_g = \frac{2V_g{}^i}{\hbar v} = \frac{2\pi^2\hbar^2 n}{\Omega m^2 v^2} \int_0^{2\pi} \int_0^{S_m} [\Delta f(\boldsymbol{S}) \, \Delta f^*(\boldsymbol{S} - \boldsymbol{g}) \cdot \exp\{-2\pi i \boldsymbol{g} \cdot \boldsymbol{r}_i\} + \text{c.c.}] S \, dS \, d\varphi . \qquad (10)$$

The number of cases to which these equations can applied is vast, and we can only indicate the magnitude of the results obtained for a particular case, chosen because of the availability of the appropriate data.

For the case of a substitutional atom A placed in a host lattice B, we can (neglecting lattice binding, the effect of screening, and size effects) replace $\Delta f(\boldsymbol{S})$ by $f_A(S) - f_B(S)$, the difference of the atomic scattering amplitudes. In Cu 10 atomic % Al we calculate, in this approximation, a value of $\Lambda = 18{,}000$

**** The variation of the secondary electron emission with incident electron angle in the energy range 200 – 2000 eV has been shown [39] to be dependent on the diffraction conditions of the incident electrons. Some of this may be due to anomalous absorption effects.

Å at 100 keV. At lower energies it is again necessary to use phase shift formulae, and one readily obtains the result:

$$\Delta\mu_g = \frac{4\pi\hbar^2 n}{\Omega\, m_0^2\, v^2} \sum_{l=0}^{\infty} (2l+1)\, P_l(\cos 2\Theta_B) \cdot \sin^2(\delta_l^A - \delta_l^B) \qquad (11)$$

where Θ_B is the Bragg angle for the reflection g. With $P_l(\cos 2\Theta_B) = 1$, Eq. (11) gives the value of μ_0 and hence Λ. Using the phase shift data previously mentioned, we thus obtain for disorder scattering in the same Cu-Al alloy values of $\Lambda = 25$ Å and 45 Å at 27 eV and 109 eV respectively. In the latter case we also find $\Delta\mu_{111} \sim 0.6\,\mu_0$ so that for some Bloch waves the mean free path may be considerably reduced by anomalous absorption effects.

In an attempt to improve this calculation, we can estimate the importance of screening effects by using a simple screened impurity potential

$$V = \Delta z\, e^2 \exp\{-q\, r\}/r$$

from which we obtain in the Born approximation,

$$\Delta f(\mathbf{S}) = 2\,\Delta Z/a_{\mathrm{H}}\,(4\pi^2 S^2 + q^2)\,.$$

With this value of $\Delta f(\mathbf{S})$ Eq. (9) can readily be integrated to obtain a good approximation

$$\frac{1}{\Lambda} = \frac{4\pi\, n\, (\Delta Z)^2}{\Omega\, (q\, a_{\mathrm{H}})^2\, m_0^2\, v^2}\,. \qquad (12)$$

Putting $q\, a_{\mathrm{H}} = 1$, we obtain for the CuAl alloy discussed above a value of Λ ranging from about 25 Å at 50 eV, to 5×10^4 Å at 100 keV. Clearly at high energies the valence electron screening effects are less significant and the majority of the scattering occurs because of the difference in the atomic cores. At low energies a consistent screened potential is needed, but it appears that in the very low energy region, where the disorder scattering mean free path is still decreasing, that the disorder contribution may be significant.

Disorder effects in other alloys may well be larger than the one we have considered here. In more concentrated alloys, (provided the scattering centres are still independent), the factor n in Eqs. (9) – (12) should be replaced by $n(1-n)$. In the case of interstitial alloys, $\Delta f(\mathbf{S})$ must include the atomic scattering factor $f_i(S)$ of the impurity as well as the effects due to the displacements of surrounding atoms. As was pointed out by HALL et al. [40] the effect of interstitials may be to make a negative contribution to $\Delta\mu_g$ since the factor $\exp\{-2\pi i\, \boldsymbol{g}\cdot\boldsymbol{r}_i\}$ in Eq. (10) will no longer be unity if the interstitial lies between the reflecting planes (g) considered.

Discussion

Figures 3, 4 and 5 indicate that the electronic contribution to Λ is important at almost all energies and that thermal diffuse scattering must also be considered at all energies above 200 eV particularly in heavy materials with low Debye temperatures. Anomalous absorption effects may be significant in this energy range. Our calculations show that if more accurate estimates are to be obtained the available data must be improved in a number of respects. For the electronic contributions a more complete knowledge of $\varepsilon(q, \omega)$ is essential and for the thermal diffuse scattering better atomic scattering data in the range 100 eV to 10 keV are needed. In alloys the disorder scattering is probably a small effect except at very low energies but in this range a proper screened scattering potential is required. Between 50 and 500 eV the resultant mean free path from all processes is reasonably constant between 5 and 8 Å for the metals considered. This agrees with evidence from observed diffraction peak widths in this energy range [41].

One source of absorption not considered here is the weak Bragg reflections. HALL and HIRSCH [42] considered this effect in the transmission case, defining weak beams to be those with Bragg reflection extinction distances ξ_g greater than twice the crystal thickness t. A possible alternative criterion would be to consider all reflections for which $\Lambda < 2\,\xi_g$ as weak where Λ is the mean free path allowing for all the different contributions. This is equivalent to the condition $V_0^{\mathrm{i}} \geqq 2\, V_g$ where V_g is the Fourier component of the lattice potential. It may be that all reflections meeting this condition are weak, can be treated kinematically, and contribute to absorption. At high energies this source of absorption is relatively small but it would be interesting to examine the situation in more detail at lower energies in the light of the calculations presented here.

Finally, we should mention some limitations of the optical potential. In some cases it is necessary to obtain a more complete solution for the propagation of the inelastically scattered electrons. In electron microscopy for instance, where inelastically scattered electrons may pass through the aperture and contribute to image contrast, the small-angle predominantly plasmon-scattered component must be treated separately [43]. In the case of reflection diffraction there may be special effects with surface plasmons [44] and with long-wavelength phonons [45] which should be further investigated.

Acknowledgments

We are grateful to Dr. J. B. Pendry for a number of valuable discussions and for supplying us with his unpublished phase shift data for Cu. — R. M. Stern thanks the Science Research Council for a Visiting Fellowship.

[1] A. Sommerfeld and H. A. Bethe, Handbuch der Physik (Geiger/Scheel), Springer-Verlag, Berlin, Vol. 24/2.

[2] M. von Laue, Ann. Physik Leipzig **26**, 55 [1936].

[3] J. W. Harding, Phil. Mag. **23**, 271 [1937].

[4] P. A. M. Dirac, Quantum Mechanics, Clarendon Press, Oxford 1930, p. 194.

[5] J. C. Slater, Phys. Rev. **51**, 840 [1937].

[6] K. Molière, Ann. Phys. Leipzig (5) **34**, 461 [1939].

[7] G. Honjo and K. Mihama, J. Phys. Soc. Japan **9**, 184 [1954].

[8] K. Kohra and H. Watanabe, J. Phys. Soc. Japan **16**, 580 [1961].

[9] H. Hashimoto, A. Howie, and M. J. Whelan, Proc. Roy. Soc. London A **269**,80 [1962].

[10] P. Goodman and G. Lehmpfuhl, Acta Cryst. **22**, 14 [1967].

[11] H. Yoshioka, J. Phys. Soc. Japan **12**, 618 [1957].

[12] M. J. Whelan, J. Appl. Phys. **36**, 2099 [1965].

[13] H. Yoshioka and Y. Kainuma, J. Phys. Soc. Japan **17**, B II, 134 [1962].

[14] M. J. Whelan, J. Appl. Phys. **36**, 2103 [1965].

[15] C. R. Hall and P. B. Hirsch, Proc. Roy. Soc. London A **286**, 158 [1965].

[16] K. Kambe and K. Molière, Adv. in Structure Research by Diffraction Methods, **3**, 53 [1970] (Pergamon Press).

[17] H. A. Bethe, Ann. Phys. Leipzig (4) **87**, 55 [1928].

[18] R. M. Stern and H. Taub, Critical Reviews in Solid State Sciences, **1**, 221 [1970].

[19] J. B. Pendry, J. Phys. C. (Proc. Phys. Soc.) **2**, 2273 [1969].

[20] C. B. Duke and C. W. Tucker, Jun., Surface Sci. **15**, 231 [1969].

[21] J. A. Strozier and R. O. Jones, Phys. Rev. **B 3**, 3228 [1971].

[22] Y. Kamiya and R. Uyeda, J. Phys. Soc. Japan **16**, 1361 [1961].

[23] F. Lenz, Z. Naturforsch. **9 a**, 185 [1954].

[24] J. J. Quinn, Phys. Rev. **126**, 1453 [1962].

[25] B. I. Lundqvist, Phys. Stat. Sol. **32**, 273 [1969].

[26] G. Radi, Z. Phys. **213**, 244 [1968].

[27] J. Daniels, C. V. Festenberg, H. Raether, and K. Zeppenfeld, Springer Tracts in Modern Physics **54**, 77 [1970].

[28] M. Ichikawa and Y. H. Ohtsuki, J. Phys. Soc. Japan **27**, 953 [1969].

[29] K. Hirabayashi, J. Phys. Soc. Japan **30**, 211 [1971].

[30] A. Ignatjevs, J. B. Pendry, and T. N. Rhodin, Phys. Rev. Letters **26**, 189 [1971].

[31] P. A. Dolye and P. S. Turner, Acta Cryst. **A 24**, 390 [1968].

[32] C. J. Humphreys and P. B. Hirsch, Phil. Mag. **18**, 115 [1968].

[33] E. C. Snow, Phys. Rev. **158**, 683 [1967].

[34] J. B. Pendry, J. Phys. C. (Proc. Phys. Soc.) **4**, 2501 [1971].

[35] G. Capart, Surface Sci. **26**, 429 [1971].

[36] J. Kessler and H. Lindner, Z. Phys. **183**, 1 [1965].

[37] G. Holzwarth and H. J. Meister, Nucl. Phys. **A 59**, 56 [1964].

[38] D. S. Boudreaux and V. Hoffstein, Phys. Rev. **B 2**, 3013 [1970].

[39] H. Taub, R. M. Stern, and V. F. Dvoryankin, Phys. Stat. Sol. **33**, 573 [1969].

[40] C. R. Hall, P. B. Hirsch, and G. R. Booker, Phil. Mag. **14**, 979 [1966].

[41] R. M. Stern and F. Balibar, Phys. Rev. Lett. **25**, 1338 [1970].

[42] C. R. Hall and P. B. Hirsch, Phil. Mag. **12**, 539 [1965].

[43] A. Howie, Proc. Roy. Soc. London A **271**, 268 [1963].

[44] M. Sunjic and A. A. Lucas, Phys. Rev. **B 3**, 719 [1971].

[45] V. Heine and J. B. Pendry, Phys. Rev. Letters **22**, 1003 [1969].