On the Reflection of Electrons by Metallic Crystals

By L. A. MacColL

This paper gives the results of some calculations of the reflection coefficient for electrons incident normally on a plane face of a metallic crystal. The physical situation is treated as being one-dimensional; and it is assumed that the potential energy of an electron is a sinusoidal function of distance inside the crystal, and obeys the classical image force law outside the crystal. The reflection coefficient is computed as a function of the energy of the incident electrons, over the range from 0 to 20 electron volts, for a variety of values of the parameters which define the model of the crystal.

1. Foreword

THE work which is presented in this paper was undertaken as a result of conversations had with Dr. C. J. Davisson at various times during the years 1938 and 1939, when he was investigating the reflection of electrons impinging on the surface of a metallic crystal. The results for a simple special case of the general problem were published in 1939[1]. Thereafter the work on the general problem continued intermittently, and it was almost completed by the early part of 1942, when it was brought to a halt by the onset of wartime activities. Since then nothing has been done on the problem, and the results already obtained have never been published *in extenso*. However, C. Herring and M. H. Nichols have included an illuminating discussion of some of the more significant of the results in their recent monograph on thermionic emission[2].

Although the intervening years, by bringing new problems in physics to the fore, have caused this work to lose some of the interest which it possessed at the time it was being done, it still seems to be worth while to put the full results upon record. The present occasion, when his friends and former colleagues are celebrating Dr. Davisson's seventieth birthday, is an especially appropriate one for this purpose.

2. Formulation of the Problem

We consider electrons moving with energy E and impinging on a plane face of a metallic crystal. (Fig. 1.) According to quantum mechanics there is certain probability R, generally neither 0 nor 1, that an electron will be reflected by the crystal, and caused to move backwards toward the source; and there is the complementary probability $1 - R$ that the electron will

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[1] *Physical Review*, v. 56, pp. 699–702. This paper will be referred to henceforth as [LAM, 1939].
[2] *Reviews of Modern Physics*, v. 21, pp. 185–270 (1949).

penetrate the crystal, and flow away through the remainder of the circuit. We call R the *reflection coefficient*, and we can define it alternatively as the ratio of the intensity of the reflected electron beam to the intensity of the incident beam.

We wish to calculate R as a function of E. In order to be able to do this effectively, it is necessary to idealize the actual physical situation quite drastically. (However, the idealization which we shall use preserves what seem to be the most important features of the physical situation.) On the other hand, once the idealization has been set up, the mathematical calculations themselves will be carried through without approximations[3]. Hence,
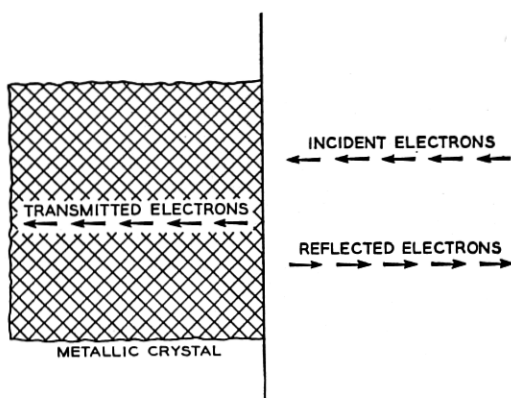

Fig. 1—Reflection of an electron beam by a crystal. (Schematic representation).

any discrepancies between the theoretical results and the results of experiment are to be attributed to the inadequacy of the model, and not to illegitimate steps in the mathematical work.

Our idealization of the physical situation can be described in the form of the three following assumptions:

Assumption I. The problem may be treated as one concerning one-dimensional motion of electrons. Thus, we set up a rectangular coordinate system in space; and we assume that the crystal occupies the half-space $x < 0$, and that all of the point functions with which we are concerned depend solely upon the coordinate x.

Assumption II. There exists a function $V(x)$, such that an electron at the point x has potential energy $V(x)$; and the behavior of an electron is governed by the Schrödinger wave equation

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[3] Except, of course, simple arithmetical approximations, such as are involved in almost all calculations.

$$\frac{d^2\psi}{dx^2} + k^2 [E - V(x)]\psi = 0. \tag{1}$$

(Here $k^2 = 8\pi^2 m/h^2$, where h is Planck's constant, and m is the mass of an electron.) This assumption deals in a summary way with various complicated processes involving electrons in crystals. Discussions of the validity of the assumption are to be found in various works on the electron theory of metals.
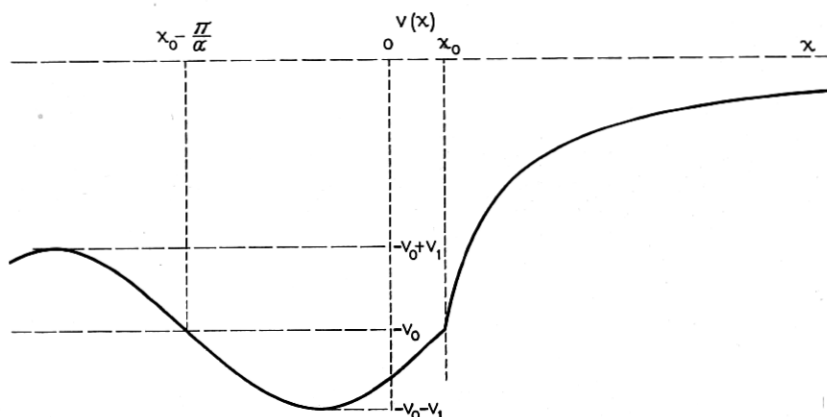

Fig. 2—Assumed potential energy as a function of the coordinate x.

Assumption III. Specifically, the function $V(x)$ is given by the formulae

$$
\begin{aligned}
V(x) &= -V_0 + V_1 \sin \alpha(x - x_0), & x &\leq x_0 \\
&= -\epsilon^2/(4x), & x &\geq x_0 \\
x_0 &= \epsilon^2/(4V_0),
\end{aligned}
\tag{2}
$$

where ϵ is the absolute value of the electronic charge, and V_0, V_1 and α are suitable non-negative constants. (A graph of this function $V(x)$ is shown in Fig. 2.) According to this assumption, an electron in the region $x > x_0$ is subjected to the classical image force. This is known to be in good agreement with the facts, at least if x is not too small.* Also, according to the assumption, the potential energy of an electron in the depths of the crystal is a periodic point function with a negative mean value. This part of the assumption is as correct as any assumption can be which attempts to account for the complicated actual processes in terms of a potential energy function. However, our particular choice of a periodic function is based largely upon mere considerations of mathematical convenience. Finally, we

* See Herring and Nichols, footnote 2, p. 245 et seq.

observe that our $V(x)$ is continuous, as physical considc...tions indicate that it should be.

We can now state the mathematical problem befcre us in the following terms:

$V(x)$ being defined by (2), we are to obtain a solution $\psi(x)$ of (1) satisfying the following conditions:

(a) In the region $x > x_0$ the function $\psi(x)$ exp $(-2\pi iEt/h)$ represents an incident beam of electrons moving toward the left, and a reflected beam of electrons moving toward the right.

(b) In the region $x < x_0$ the average electron flow, if it is not zero, is directed toward the left.

(c) The function $\psi(x)$ and its derivative $\psi'(x)$ are everywhere continuous.

Having obtained such a solution $\psi(x)$, we are then to compute the ratio of the intensity of the reflected electron beam to the intensity of the incident beam. In particular, we are to study the dependence of this ratio upon the quantities E, V_0, and V_1.

The paper [LAM, 1939] already referred to dealt with the special case in which $V_1 = 0$, i.e. the case in which $V(x)$ is assumed to be constant in the region $x \leq x_0$. Consequently, we are now concerned chiefly with the cases in which $V_1 > 0$.

3. Generalities Concerning the Calculation of R

In the region $x \geq x_0$ the wave equation (1) takes the form

$$\frac{d^2\psi}{dx^2} + k^2\left[E + \frac{\epsilon^2}{4x}\right]\psi = 0.$$

The general solution of this equation is of the form

$$\psi(x) = A\psi_1(x) + B\psi_2(x),$$

where A and B are arbitrary constants, and $\psi_1(x)$ and $\psi_2(x)$ are two particular solutions which we choose so that the functions $\psi_1(x)$ exp $(-2\pi iEt/h)$ and $\psi_2(x)$ exp $(-2\pi iEt/h)$ represent beams of electrons, of unit intensity, moving to the left and right, respectively.

In the region $x \leq x_0$ the wave equation takes the form

$$\frac{d^2\psi}{dx^2} + k^2[E + V_0 - V_1 \sin \alpha(x - x_0)]\psi = 0. \tag{3}$$

We are concerned with a solution of this equation of the form

$$\psi(x) = C\psi_3(x),$$

where C is a constant, and $\psi_3(x)$ is a particular solution such that the func-

tion $\psi_3(x) \exp(-2\pi i Et/h)$ represents a state in which the average flow of electrons in the crystal either vanishes or is directed toward the left.

The actual forms of the functions $\psi_1(x)$, $\psi_2(x)$, $\psi_3(x)$ will be discussed presently.

Now the continuity of the functions $\psi(x)$ and $\psi'(x)$ gives us the system of equations

$$A\psi_1(x_0) + B\psi_2(x_0) = C\psi_3(x_0)$$
$$A\psi_1'(x_0) + B\psi_2'(x_0) = C\psi_3'(x_0),$$

from which we can calculate the ratio B/A in terms of the $\psi_i(x_0)$, $\psi_i'(x_0)$. Our required reflection coefficient R is $|B/A|^2$, and so we obtain the formula

$$R = \left| \frac{\psi_1'(x_0) - \dfrac{\psi_3'(x_0)}{\psi_3(x_0)} \psi_1(x_0)}{\psi_2'(x_0) - \dfrac{\psi_3'(x_0)}{\psi_3(x_0)} \psi_2(x_0)} \right|^2. \tag{4}$$

It was shown in [LAM, 1939] that the functions $\psi_1(x)$ and $\psi_2(x)$ are given by the formulae

$$\psi_1(x) = W_{\lambda,\frac{1}{4}}(\xi), \qquad \psi_2(x) = W_{-\lambda,\frac{1}{4}}(-\xi),$$

where

$$\xi = 2ikxE^{1/2}, \qquad \lambda = -ik\epsilon^2/(8E^{1/2}),$$

and the symbols $W_{\lambda,\frac{1}{4}}(\xi)$, $W_{-\lambda,\frac{1}{4}}(-\xi)$ denote the usual functions occurring in the theory of the confluent hypergeometric functions[4]. The earlier work gives us all the information concerning $\psi_1(x)$ and $\psi_2(x)$ that we shall require. Hence, in order to calculate R, we have, in effect, only to identify a suitable solution $\psi_3(x)$ of equation (3), and then to calculate $\psi_3'(x_0)/\psi_3(x_0)$.

4. THE SOLUTION OF EQUATION (3)

In order to facilitate the use of known results, it is convenient to write

$$\alpha(x - x_0) = 2z - \frac{\pi}{2}, \qquad \frac{4k^2}{\alpha^2}(E + V_0) = \theta_0^2, \qquad \frac{4k^2}{\alpha^2} V_1 = -2\theta_1.$$

Then equation (3) takes the form

$$\frac{d^2\psi}{dz^2} + (\theta_0^2 + 2\theta_1 \cos 2z)\psi = 0. \tag{3'}$$

This is one of the canonical forms of Mathieu's differential equation, for

[4] E. T. Whittaker and G. N. Watson, "Modern Analysis" (Chapter XVI), Cambridge Univ. Press, 4th Ed., 1927.

which an extensive theory exists. We shall recall a few of the chief facts brought out in this theory.†

Unless the constants θ_0 and θ_1 satisfy some one of certain special relations, the general solution of equation (3′) is of the form

$$\psi = K_1 e^{\mu z} f(z) + K_2 e^{-\mu z} f(-z),$$

where μ is a constant determined by θ_0 and θ_1, $f(z)$ is a function which is periodic with the period π, and the K's are constants of integration.

In certain ranges of values of the θ's, the constant μ is real, and in other ranges it is pure imaginary. When μ is real we can obviously take it to be positive; and then, in order that $\psi_3(x)$ may be bounded in the range $x < x_0$, we must choose $\psi_3(x)$ to be the function $e^{\mu z} f(z)$. When μ is pure imaginary, we can take it to be $i\,|\,\mu\,|$; and then, in order that $\psi_3(x)$ shall represent a state in which the flow of electrons is to the left in the crystal, we must choose $\psi_3(x)$ to be the function $e^{-\mu z} f(-z)$.

When μ is pure imaginary we have a non-vanishing flow of electrons to the left in the crystal. Consequently, the intensity of the reflected beam must be less than the intensity of the incident beam. Hence, under this condition we must have $R < 1$. On the other hand, when μ is real there is no average electron flow in the crystal. Consequently, under this condition the intensities of the incident and reflected beams must be equal, so that $R = 1$. These considerations point to the importance of discussing, first of all, the conditions under which μ is real or pure imaginary.

Figure 3 shows a well known diagram, modified slightly to suit our present purposes[5]. Here θ_0^2 and θ_1 are taken to be rectangular coordinates of a point in a plane, and the plane is divided into regions of two kinds (shaded and unshaded) by a system of curves. If the point (θ_0^2, θ_1) is in the interior of one of the shaded regions, the above μ is real; if the point is in the interior of one of the unshaded regions, μ is pure imaginary. (If (θ_0^2, θ_1) lies exactly on the boundary of one of the regions, we have a somewhat more complicated situation, which we do not need to consider here.) This diagram enables us easily to determine, for any fixed values of V_0 and V_1, the ranges of values of E in which we have $R = 1$. We shall call these ranges of values of E the *diffraction bands*.

Now our problem has been reduced to that of computing R for values of E which do not lie in diffraction bands. In treating this phase of the subject we shall follow the course of the actual calculations, without any examination of ways in which the work might have been done more efficiently.

† See, for instance, E. T. Whittaker and G. N. Watson, footnote 4, Chapter XIX.
[5] See, for instance, N. W. McLachlan, "Theory and Application of Mathieu Functions" (p. 40), Oxford University Press, 1947.

Of the many methods which have been devised for finding solutions of Mathieu's differential equation, the one which is conceptually simplest is that due to Bruns. This method can be described as follows:
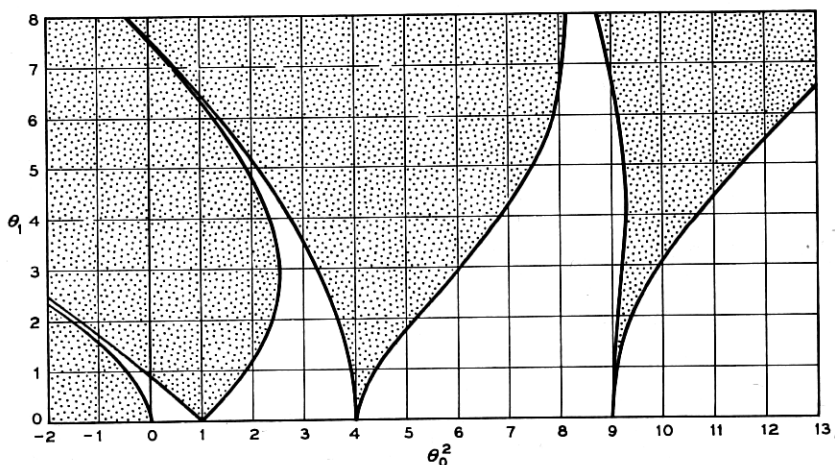

Fig. 3—Stability diagram for Mathieu's differential equation.

Under the transformation

$$\psi = \exp \int_{z_0}^{z} \varphi(z) dz$$

the Mathieu equation $(3')$ goes over into the Riccati equation

$$\frac{d\varphi}{dz} + \varphi^2 + \theta_0^2 + 2\theta_1 \cos 2z = 0. \tag{5}$$

We seek a solution of this equation in the form of a power series in the parameter θ_1, say

$$\varphi(z) = \varphi_0(z) + \theta_1 \varphi_1(z) + \theta_1^2 \varphi_2(z) + \cdots ,$$

and we easily find that the functions $\varphi_0(z)$, $\varphi_1(z)$, $\varphi_2(z)$, ... must satisfy the differential equations

$$\begin{aligned}
&\varphi_0' + \varphi_0^2 + \theta_0^2 = 0, \\
&\varphi_1' + 2\varphi_0\varphi_1 + 2 \cos 2z = 0, \\
&\varphi_2' + 2\varphi_0\varphi_2 + \varphi_1^2 = 0, \\
&\varphi_3' + 2\varphi_0\varphi_3 + 2\varphi_1\varphi_2 = 0, \\
&\varphi_4' + 2\varphi_0\varphi_4 + 2\varphi_1\varphi_3 + \varphi_2^2 = 0, \\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots
\end{aligned} \tag{6}$$

Obviously, in order that we shall get the solution which we require, $\varphi(z)$ must reduce to $-i\theta_0$ when $V_1 = 0$. Also $\varphi(z)$ must be periodic with the period π. These conditions, together with the equations (6), suffice to determine $\varphi_0(z)$, $\varphi_1(z)$, $\varphi_2(z)$, $\cdots$ successively and uniquely. We easily obtain the results:

$$\varphi_0(z) = -i\theta_0,$$

$$\varphi_1(z) = -\frac{1}{2i}\left[\frac{e^{2iz}}{1-\theta_0} - \frac{e^{-2iz}}{1+\theta_0}\right],$$

$$\varphi_2(z) = \frac{1}{8i}\left[\frac{e^{4iz}}{(1-\theta_0)^2(2-\theta_0)} + \frac{2}{(1-\theta_0^2)\theta_0} - \frac{e^{-4iz}}{(1+\theta_0)^2(2+\theta_0)}\right]$$

$$\varphi_3(z) = -\frac{1}{16i}\left[\frac{e^{6iz}}{(1-\theta_0)^3(2-\theta_0)(3-\theta_0)} + \frac{(4-3\theta_0)e^{2iz}}{(1-\theta_0)^3(1+\theta_0)\theta_0(2-\theta_0)}\right.$$
$$\left. + \frac{(4+3\theta_0)e^{-2iz}}{(1+\theta_0)^3(1-\theta_0)\theta_0(2+\theta_0)} - \frac{e^{-6iz}}{(1+\theta_0)^3(2+\theta_0)(3+\theta_0)}\right],$$

$$\varphi_4(z) = \frac{1}{128i}\left[\frac{(11-5\theta_0)e^{8iz}}{(1-\theta_0)^4(2-\theta_0)^2(3-\theta_0)(4-\theta_0)}\right.$$
$$+ \frac{4(15-18\theta_0+5\theta_0^2)e^{4iz}}{(1-\theta_0)^4(1+\theta_0)(2-\theta_0)^2(3-\theta_0)\theta_0} - \frac{2(8-35\theta_0^2+15\theta_0^4)}{(1-\theta_0^2)^3(4-\theta_0^2)\theta_0^3}$$
$$+ \frac{4(15+18\theta_0+5\theta_0^2)e^{-4iz}}{(1+\theta_0)^4(1-\theta_9)(2+\theta_0)^2(3+\theta_0)\theta_0}$$
$$\left. - \frac{(11+5\theta_0)e^{-8iz}}{(1+\theta_0)^4(2+\theta_0)^2(3+\theta_0)(4+\theta_0)}\right].$$

The functions $\varphi_5(z)$ and $\varphi_6(z)$ have been computed also; but, because of their complexity, they will not be exhibited here.

It is easily found that the expression $\psi_3'(x_0)/\psi_3(x_0)$ appearing in equation (4) has the value $\varphi(\pi/4)(\alpha/2)$ in terms of our present notation[6].

In principle we now have all the information we need to calculate the reflection coefficient R. Furthermore, our experience showed that it is quite easy to compute R by this method, provided that the value of E does not lie too near an edge of a diffraction band. However, Brun's method proved to be unsuitable for calculating values of R for values of E in the neighborhood of a diffraction band edge, and we were forced to seek another method to obtain these values. After some tentative work with other methods, we

[6] We must take account of the fact that the symbols $\psi(x)$ and $\psi(z)$, which we are using for convenience, do not represent merely the same function with different arguments. In fact, after the change of the independent variable from x to z we have the following relation between the old and new ψ's: $[\psi(x)]_{\text{old}} = [\psi(x_0 + 2z/a - \pi/2a)]_{\text{old}} = [\psi(z)]_{\text{new}}$.

settled upon a method due to Whittaker, and this was used to complete the calculations.

Whittaker's method is described briefly in Whittaker and Watson's "Modern Analysis," 4th Edition, p. 424. The method is developed more fully in papers by Ince[7]. We shall confine ourselves here to some summary indications of the nature of the method.

The method leads to representations of the solutions of Mathieu's equation by formulae which differ in structure depending upon the part of the (θ_0^2, θ_1) plane in which we are working. We shall give the formulae suitable for use in the neighborhood of the point $\theta_0^2 = 1, \theta_1 = 0$; the formulae for use in other parts of the plane are given by Ince.

Given the values of θ_0^2 and θ_1, we first determine a number σ by means of the implicit equation

$$\theta_0^2 = 1 + \theta_1 \cos 2\sigma + \frac{\theta_1^2}{8} (-2 + \cos 4\sigma) - \frac{\theta_1^3}{64} \cos 2\sigma$$
$$+ \frac{\theta_1^4}{512} \left(\frac{32}{3} - 11 \cos 4\sigma \right) + \cdots .$$

Then we seek a solution of equation (3′) in the form

$$\psi = e^{\mu z} \sum_{n=0}^{\infty} \{a_{2n+1} \cos[(2n + 1)z - \sigma] + b_{2n+1} \sin[(2n + 1)z - \sigma]\},$$

where μ, the a's, and the b's are constants. We substitute the expression for ψ into the differential equation, and determine values of the constants by imposing the condition that the resulting relation shall be an identity in z. After some rather intricate algebraic manipulations we finally arrive at the following results:

$$\mu = \frac{\theta_1}{2} \sin 2\sigma - \frac{3\theta_1^3}{128} \sin 2\sigma - \frac{3\theta_1^4}{1024} \sin 4\sigma + \cdots$$

$$a_1 = 0, \qquad b_1 = 1$$

$$a_3 = \frac{3\theta_1^2}{64} \sin 2\sigma + \frac{3\theta_1^3}{512} \sin 4\sigma + \frac{\theta_1^4}{8^4} \left(-\frac{274}{9} \sin 2\sigma + 9 \sin 6\sigma \right) + \cdots$$

$$a_5 = \frac{14\theta_1^3}{(8^3)(9)} \sin 2\sigma + \frac{44\theta_1^4}{(27)(8^4)} \sin 4\sigma + \cdots$$

$$a_7 = \frac{35\theta_1^4}{(108)(8^4)} \sin 2\sigma + \cdots$$

7 *Monthly Notices, Royal Astronomical Society of London:* v. 75, pp. 436–448; v. 76, pp. 431–442.

$$a_9 = O(\theta_1^5)$$

$$b_3 = \frac{\theta_1}{8} + \frac{\theta_1^2}{64} \cos 2\sigma + \frac{\theta_1^3}{8^3}\left(-\frac{14}{3} + 5 \cos 4\sigma\right)$$

$$+ \frac{\theta_1^4}{8^4}\left(-\frac{74}{9} \cos 2\sigma + 7 \cos 6\sigma\right) + \cdots$$

$$b_5 = \frac{\theta_1^2}{192} + \frac{4\theta_1^3}{(9)(8^3)} \cos 2\sigma + \frac{\theta_1^4}{(3)(8^4)}\left(\frac{82}{9} \cos 4\sigma - \frac{155}{18}\right) + \cdots$$

$$b_7 = \frac{\theta_1^3}{(18)(8^3)} + \frac{\theta_1^4}{(12)(8^4)} \cos 2\sigma + \cdots$$

$$b_9 = \frac{\theta_1^4}{(180)(8^4)} + \cdots$$

. . . .

The calculated terms which are exhibited here enable us to calculate the solution $\psi(z)$ to a certain accuracy, and this accuracy proved to be sufficient for our purposes.

Although this method is very complicated analytically, it was found to be quite convenient for purposes of numerical calculation.

5. THE REFLECTION COEFFICIENT FOR LARGE VALUES OF E

This work is concerned chiefly with the reflection coefficient for small values of E (actually up to 20 electron volts). However, it is interesting that we can obtain a simple approximate formula for R for indefinitely large values of E in the intervals between the diffraction bands.

For this purpose we go back to Brun's method, and we write the dependent variable in equation (5) in the form $\varphi = -i\theta_0 + \omega$. We find that the new dependent variable ω satisfies the equation

$$\frac{d\omega}{dz} - 2i\theta_0\omega + \omega^2 + 2\theta_1 \cos 2z = 0,$$

and we seek a solution of this equation in the form

$$\omega := \omega_0(z) + \frac{\omega_1(z)}{\theta_0} + \frac{\omega_2(z)}{\theta_0^2} + \cdots.$$

The functions $\omega_n(z)$ are easily computed, and we finally arrive, in an entirely straight-forward way, at the result

$$\varphi(\pi/4) = -i\theta_0 + \frac{\theta_1}{\theta_0^2} + \frac{\theta_1}{\theta_0^4} + \cdots. \tag{7}$$

In [LAM, 1939] we derived an approximate formula for R when E is large for the case in which $V_1 = 0$. The work involved in that derivation, together with the equation (7), enables us to obtain the desired formula by a simple calculation. The result obtained is the following:

$$R \doteq \frac{V_0^4}{4\epsilon^4 k^2 E^3}\left[1 - \frac{\alpha\epsilon^2 V_1}{4V_0^2}\right]^2. \tag{8}$$

The range of validity of the approximate formula (8) has not been determined. The nature of the derivation, and also the form of the result, leads us to suspect that the approximation is good only so long as the ratio V_1/V_0 does not exceed some bound depending upon the other quantities entering into the expression for R. The approximation certainly breaks down when V_1/V_0 reaches the value $4V_0/(\alpha\epsilon^2)$. However, this value is well above any of the values with which we deal with in this work. Consequently, we suspect that the formula can be used, to extrapolate our calculations of R to higher values of E, without serious danger of error in the cases which we consider here.

6. The Calculated Results

The reflection coefficient depends upon the independent variable E, and upon the three parameters V_0, V_1, and α. The effects upon R of taking various values of V_0 and V_1 seemed to be of greater interest than the effect of taking various values of α; and, consequently, we confined ourselves in the calculations to a single value of α, namely, $\alpha = \pi \times 10^{-8}$ cm^{-1}. This value of α makes the period of $V(x)$ in the crystal equal to 2×10^{-8} cm.

We took six values of V_0, proceeding in equal steps from 10 electron volts to 20 electron volts inclusive. These values adequately cover the range which is of interest in connection with actual metals.

Including the calculations reported in [LAM, 1939], we have taken, for each of the values of V_0, five values of V_1, proceeding in equal steps from 0 to 0.4 V_0. Although it is somewhat difficult to say just what value of V_1 is most appropriate to the case of a specific actual metal, it appears that these values cover the range of values of interest adequately.

The results of the calculations are shown in a self-explanatory form by the curves given in Figs. 4 to 9 inclusive. For the sake of unity, we have included the results which were previously published in [LAM, 1939].

7. Physical Discussion of the Results

The results do not call for much discussion, especially in view of the discussion which Herring and Nichols have given in the paper already referred to. However, there are a few observations which should be made.
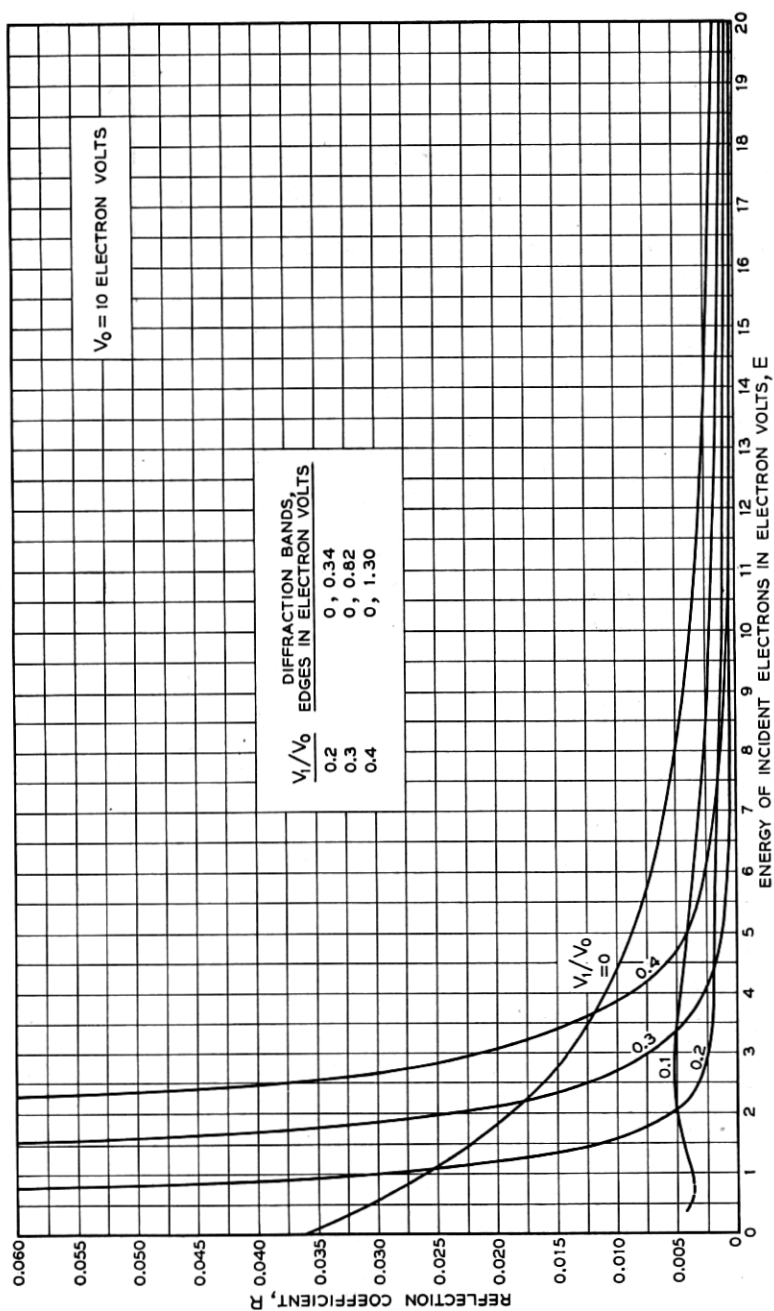
Fig. 4—Reflection coefficient as a function of energy. $V_0 = 10$ electron volts.
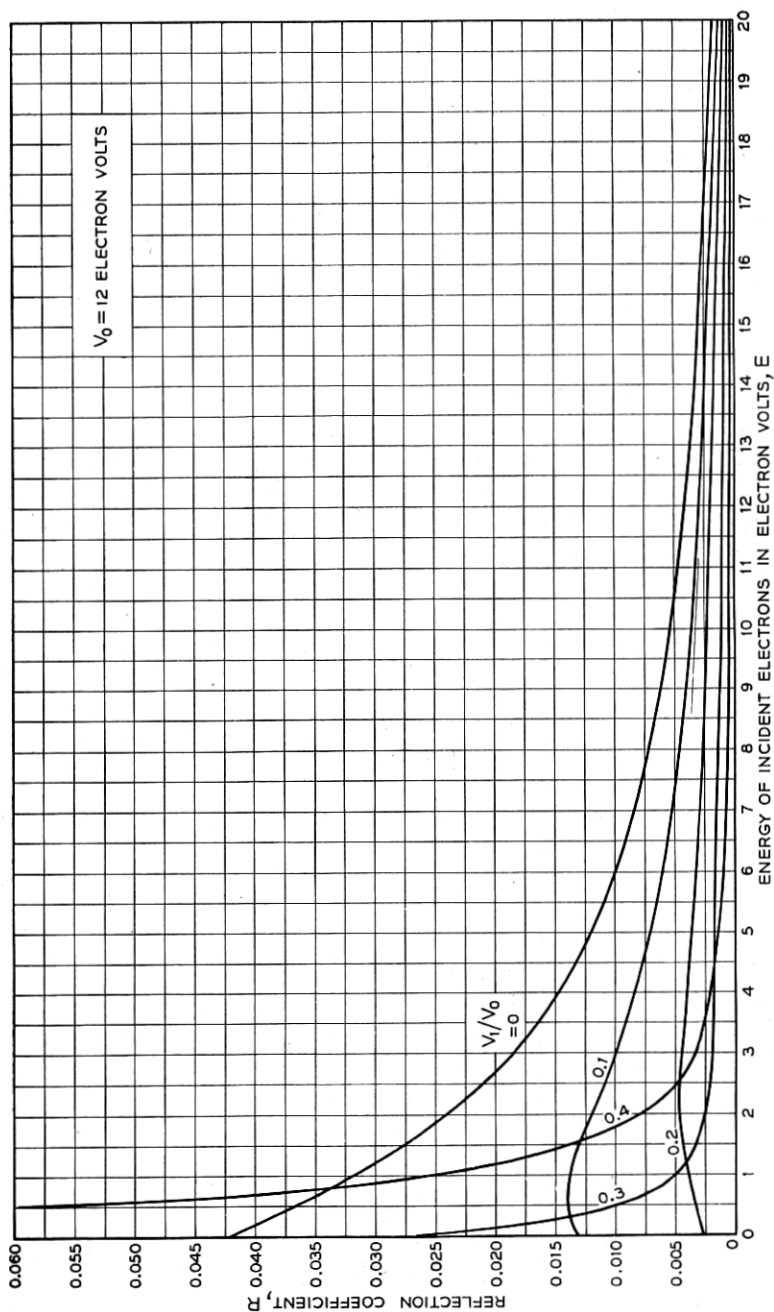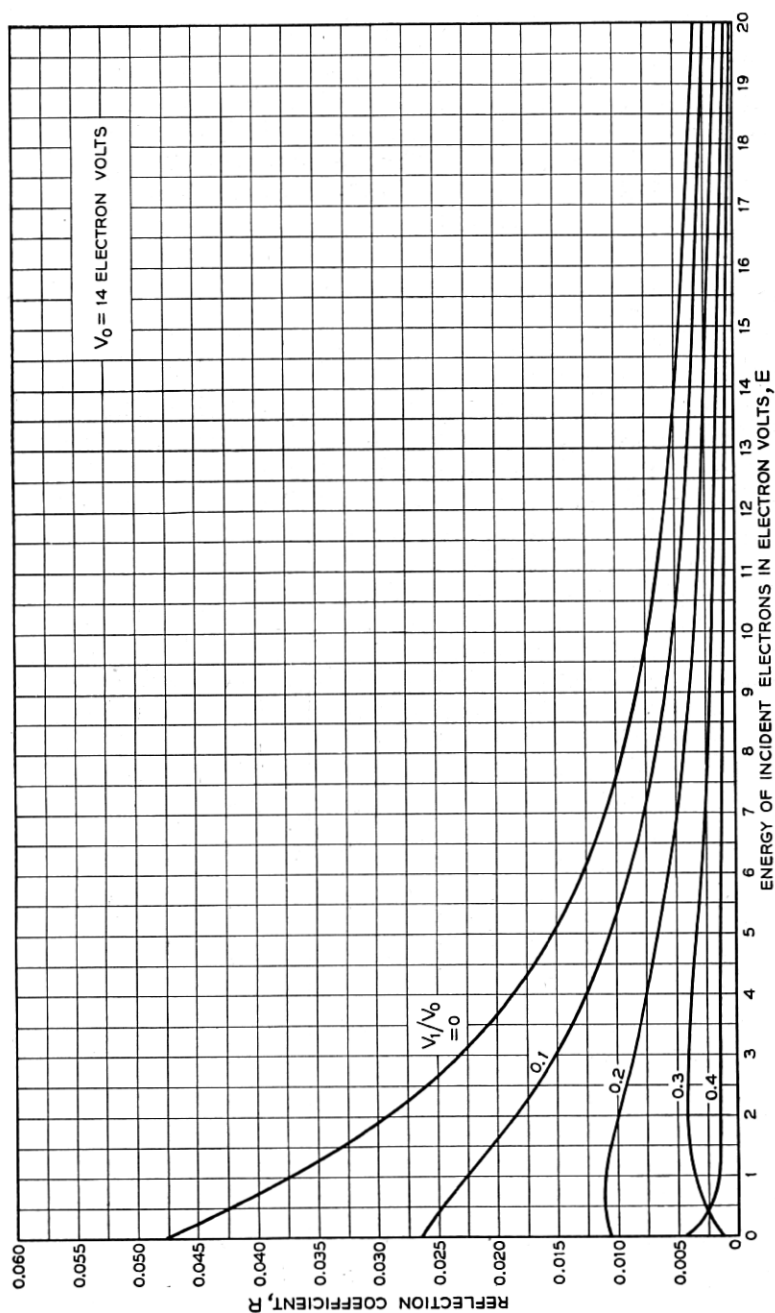
Fig. 5—Reflection coefficient as a function of energy. $V_0 = 12$ electron volts.

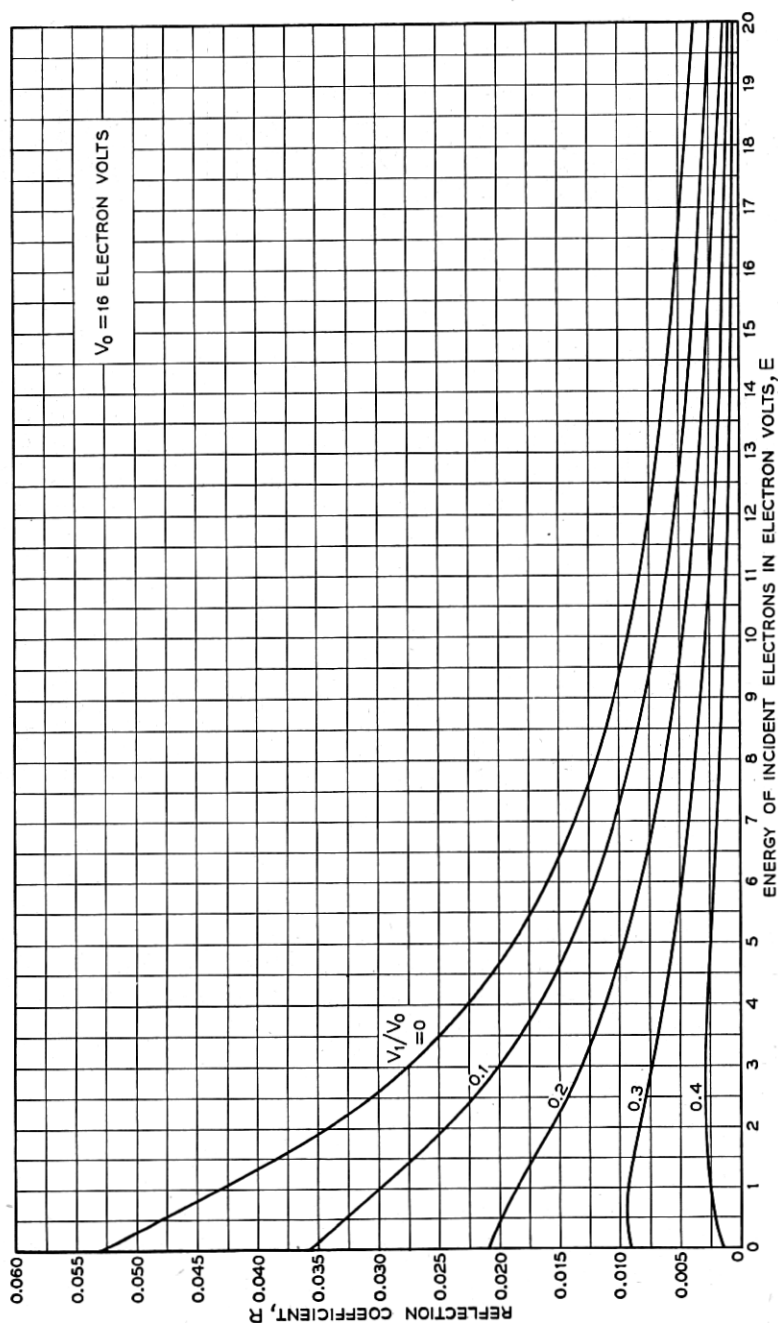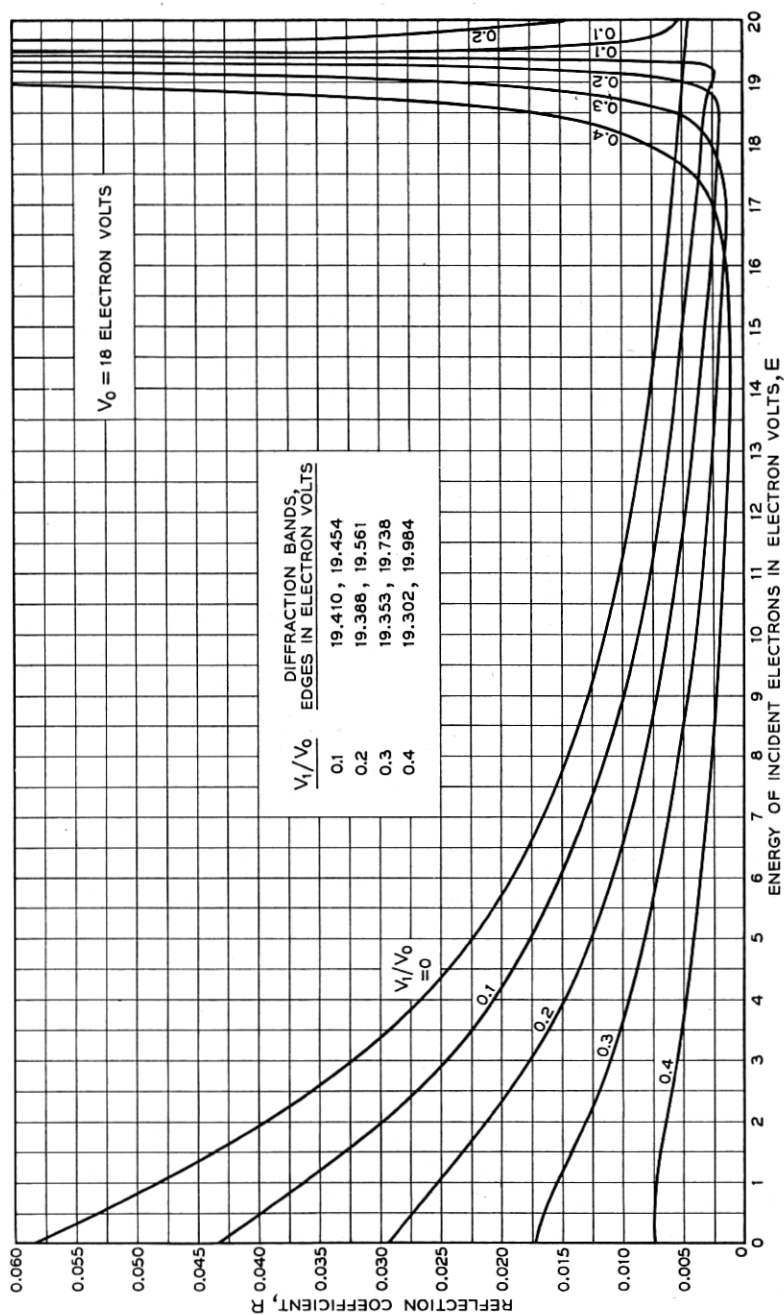Fig. 6—Reflection coefficient as a function of energy. $V_0 = 14$ electron volts.
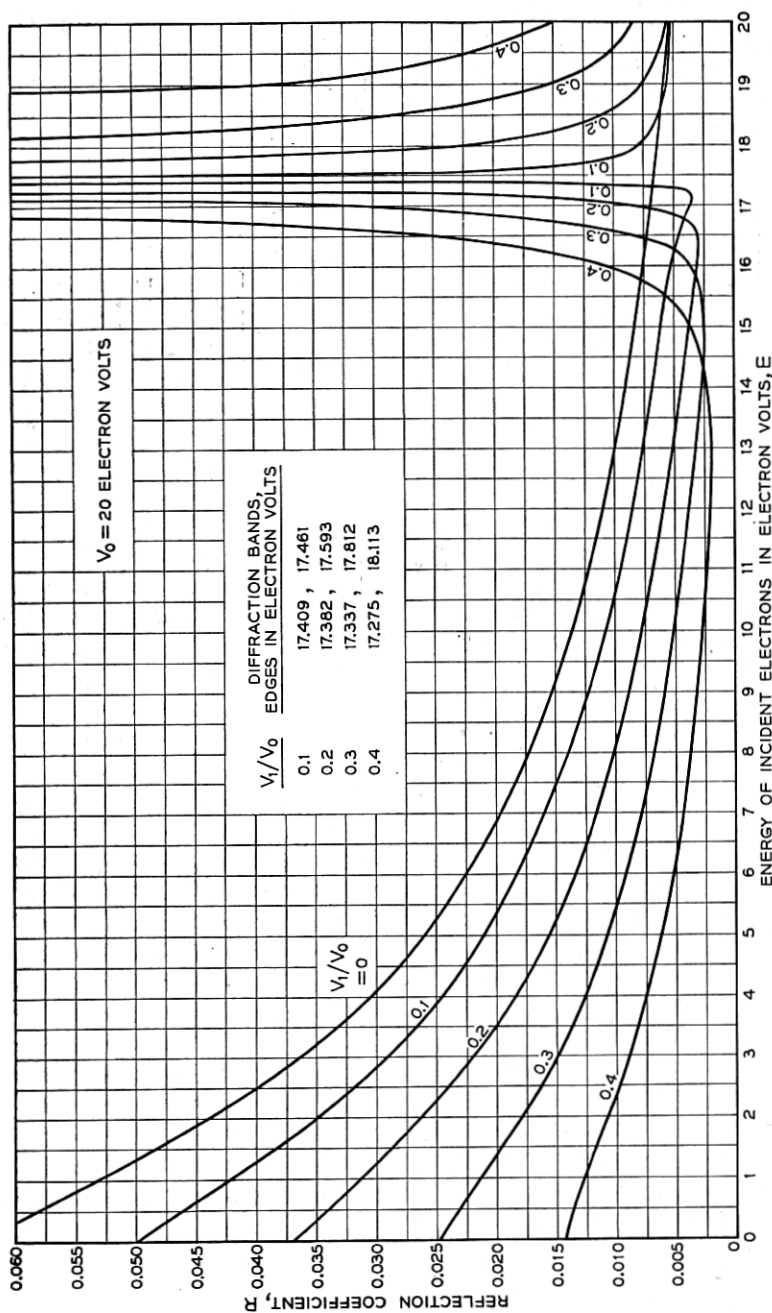
Fig. 7—Reflection coefficient as a function of energy. $V_0 = 16$ electron volts.

Fig. 8—Reflection coefficient as a function of energy. $V_0 = 18$ electron volts.

Fig. 9—Reflection coefficient as a function of energy. $V_0 = 20$ electron volts.

For fixed values of V_0 and V_1, the reflection coefficient tends to decrease with increasing E over most of the range between any two successive diffraction bands. For fixed values of V_0 and E, E being in a range between two diffraction bands, R tends to decrease with increasing V_1. This is a result which was not anticipated when the work was begun. As was expected, we find a tendency for R to increase with V_0 when E and V_1/V_0 are held fixed.

The most interesting feature of the results is the behavior of R in the neighborhoods of the edges of the diffraction bands. Unfortunately, the range of values of E considered is not great enough to reveal this behavior very completely. (The failure to consider a greater range of values of E was the result of our reluctance to embark again on the difficult numerical computations relating to the $W_{\pm\lambda,\frac{1}{2}}(\pm\xi)$ functions. Since the necessary computations had been performed earlier for values of E up to 20 electron volts, we decided, unfortunately as it now appears, to confine ourselves to this range.)

The behavior of the curves near the edges of the diffraction bands which occur in the neighborhood of $E = 19$ electron volts (when V_0 is 18 or 20 electron volts) does not require much discussion. The reader will observe a small dip in the curves for $V_1 = V_0/10$ just below these diffraction bands. The accuracy of the computations is believed to be high enough that we are justified in taking this dip to be entirely genuine.

When V_0 is 10, 12, or 14 electron volts the behavior of the curves for values of E in the neighborhood of zero is rather complicated. Herring and Nichols consider this behavior to be one of the most significant features of the results, and they have given a full discussion of it from the physical point of view.* In view of the availability of their discussion, we may confine ourselves here to a few brief remarks.

In some of the cases which we are referring to now there are diffraction bands extending from $E = 0$ to certain positive values of E. (These diffraction bands are shown in a self-explanatory way in the figures.) When such a diffraction band exists the complicated behavior of R for small values of E is a result of the existence of the diffraction band, and it is comparable with the behavior of R in the upper part of the range of values of E in the case in which $V_0 = 20$ electron volts.

In the cases in which we do not have diffraction bands extending upward from $E = 0$ we have to explain the complicated behavior of R in somewhat different terms.

Assuming that we have such a case, let us momentarily ignore the fact that the physically significant values of E are non-negative, and consider E as an unrestricted real parameter. Under this convention concerning E,

* Herring and Nichols, footnote 2, pp. 248–249.

we find that there is a diffraction band lying in the range of negative values of E, and extending more or less near to the point $E = 0^8$. We shall call this a *fictitious diffraction band*. Now it is immediately clear that the complicated behavior of our curves arises from the fact that the small positive (and hence physically significant) values of E concerned are near the upper edge of the fictitious diffraction band.

[8] Specifically, what is meant is that there is such a range of values of E in which the exponent μ is real.