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64-9

MEMORANDUM REPORT
M64-14-1

UNITED STATES ARMY

FRANKFORD ARSENAL

A COMPUTER PROGRAM FOR A KRAMERS-KRONIG
TRANSFORMATION OF THE OPTICAL REFLECTIVITY

by

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OMS Code 5010.11.83800.01
DA Project 599-01-004

MAR 3 1964

December 1963

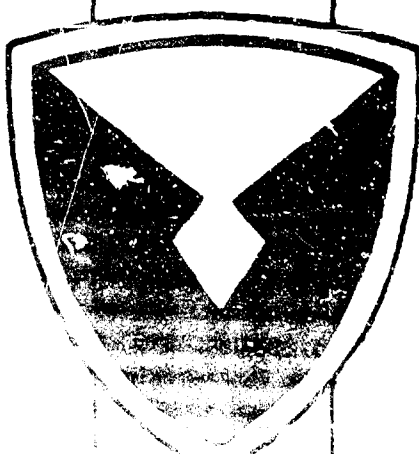
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REPORT M64-14-1



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A COMPUTER PROGRAM FOR A KRAMERS-KRONIG
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ABSTRACT

Relations involving the frequency-dependent optical constants give information on the electronic properties of solids. Power reflectivity measurements at normal incidence over a wide frequency region can be utilized in obtaining the optical constants by means of a general integral transformation known as the Kramers-Kronig transformation. A computer program based on this integral transformation has been constructed in Fortran II, version 9000, language for a Remington Rand Solid State 90 computer. The program converts experimental reflectivity measurements into parameters containing the optical constants.

A brief presentation of the electronic quasi-particle and collective excitation modes is given in terms of the optical constants. A discussion of the approximations made in putting the integrals on the computer is also given. Two tests were made to check the accuracy of the program. First, a test reflectivity function, for which the Kramers-Kronig integrals could be directly evaluated, was programmed. Then, published reflectivity measurements on copper were analyzed. The optical constants determined by the computer program were in good agreement with both the test optical constants and the previously calculated constants of copper.

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INTRODUCTION

There has been much theoretical speculation on the electronic properties of alloys. An increasing amount of research is being done on their optical properties, elastic constants, specific heat and X-ray fluorescent emission spectra in order to elucidate their band structures. Recently de Hass-van Alphen oscillations were observed in some IB-IIB alloys and other alloys.¹ The ordered beta-brass type (IB-IIB) alloys are a particularly interesting family, for they exhibit marked color changes as a function of temperature in the beta-phase and long electronic mean free paths. Muldawer² has described the color trend as going from green to yellow, to red, to gray, with increasing temperature. For example, visual observations on ordered beta CuZn reveal that it is yellow with a green tinge at -195°C , yellow gold at 28°C , and copper-red at 300°C . These striking color changes suggest that the brasses are quite amenable to optical measurements as a function of wavelength and temperature. Also, their low residual resistivities, which were observed by Rothwarf and Muldawer,³ give rise to the possibility of making Fermi surface measurements on them.

This report will be concerned with the construction of a Kramers-Kronig computer program in order to determine the electronic properties of solids from the spectral reflectivity at normal incidence. The program has been written by two of the authors* using Fortran II, revision 9000, for the Remington Rand Univac Solid State 90 computer. An analysis of reflectivity measurements on beta CuZn is given elsewhere.⁴

The power reflectivity at normal incidence is not a sensitive probe of the electronic behavior in a metal or alloy, but several relations involving the optical constants give information on the nature of the elementary electronic excitations. It is well known that electrons in a solid exhibit both individual and collective aspects.⁵ When a fast charge particle passes through a thin film, it can impart a quantum of energy to the valence electrons. The response of the electrons in the valence band(s) to the high kinetic energy of the external particle is such that an oscillation in the electron density occurs. This organized oscillation of the valence electrons as a whole is an elementary excitation of the electron gas and is known as the plasma oscillation.

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The free plasmon (the quantum of the plasma oscillation) has an energy equal to $\hbar\omega_p$ where $\omega_p^2 = 4\pi Ne^2/m$, and N and m are the electronic density and mass, respectively.

Plasmons do not influence the metallic behavior under ordinary circumstances because their excitation energies are at least a few electron volts (e.v.) greater than the kinetic energy of an electron at the Fermi surface. In those metals where the quasi-particle core excitation energies are comparable to the conduction electron plasma energies, the plasmons are severely damped and considerably shifted from their free electron values.⁶ For example, the free electron plasmon in silver should occur at approximately 9 e.v., but is actually shifted to 3.8 e.v.⁷

To first order, it has been shown that normally incident light does not excite a plasmon because the longitudinal plasma modes do not couple with the transverse photons.^{8,9} However, in the dielectric formulation of the many body problem it has been shown that, for isotropic materials, the longitudinal dielectric constant seen by a fast moving electron is equal to the transverse optical dielectric constant in the random phase approximation at wavelengths long compared to the average interelectronic spacing.⁸ Near the plasma frequency, the real part of the dielectric constant approaches zero, and the imaginary part of the inverse complex dielectric constant ($\text{Imag } 1/\epsilon$) is a maximum. It is just this latter quantity that is proportional to the rate of energy transfer from the incident charged particle to the solid in the electron characteristic energy loss experiment. Hence the plasma effects may be investigated in normal incident optical reflection and transmission experiments on account of the equivalence of the longitudinal and transverse dielectric constants. As the plasma frequency is approached from low energies, a non-interacting electron gas, due to its mass inertia, is no longer able to follow the transverse oscillations of the normal incident electromagnetic field. At this energy, a medium exhibits a characteristic crossover from highly reflective to transparent properties (neglecting interband transitions).

If a p-polarized electromagnetic wave (polarized parallel to the plane of incidence) is incident on a metallic film at an oblique angle, the surface plasma mode may be excited by the electric field component normal to the film.¹⁰ At the plasma frequency this interaction manifests itself by a dip in the transmission or a peak in the reflection. There is no such structure at the plasma energy for light polarized parallel to the plane of the film.

On the other hand, it is well known that photons excite single electron intraband and interband transitions. Structural changes in the frequency dependent absorption coefficient have been attributed to direct interband transitions at critical points in the joint density of states for the two bands participating in the transition.¹¹ These observed transitions at high symmetry points in the Brillouin zone serve as a check on the accuracy of theoretical band calculations.

The transformation of the reflectivity into the optical constants is a special case of a very general integral transformation known as the Kramers-Kronig transformation.¹² When the principles of linearity and causality apply, the real and imaginary components of a frequency dependent system are interdependent. That is to say, if the real part of a function is known over a wide region of the frequency spectrum, then the imaginary part may be found by a Fourier integral transformation of the real part, and vice versa. These dispersion relations hold for many linear systems when causality is not violated, and have been applied to such diverse fields as network theory, the quantum theory of scattering, the dielectric formulation of the many body problem, magnetic resonance, etc.

A system is linear if the response to two or more inputs is the sum or superposition of each input; e. g., if

$$\vec{D}_1 = \epsilon \vec{E}_1$$

and

$$\vec{D}_2 = \epsilon \vec{E}_2$$

then
$$\epsilon (\vec{E}_1 + \vec{E}_2) = \epsilon \vec{E} = \vec{D} = \vec{D}_1 + \vec{D}_2$$

for an isotropic medium, where $\vec{D}$ is the displacement vector, ϵ the dielectric constant, and $\vec{E}$ the electric field.

The principle of causality is concerned with a proper chronological sequencing of the input and output signals. It may be described as "no output can occur before the input"; "no scattered wave can appear until the primary wave has reached some part of the scatterer"; or "no signal can be transmitted faster than the velocity of light in a homogeneous material."¹³ Hence if

$$\vec{D}(t) = 0 \quad \text{at } t < t_0,$$

then $\vec{E}(t) = 0$ at $t < t_0$.

Also the composition of the system does not change with time; i. e., if

$$\vec{D}(t) = \epsilon \vec{E}(t)$$

then $\vec{D}(t - t_0) = \epsilon \vec{E}(t - t_0)$.

SETTING UP THE KRAMERS-KRONIG INTEGRALS

From Fresnel's equations, the reflection coefficient, r , of the electric field is complex and may be written as

$$r = \sqrt{R} e^{-i\varphi} = \sqrt{R} (\cos \varphi - i \sin \varphi) \quad (1)$$

where R is the specular power reflectivity and φ the phase angle. Both R and φ depend on the angle of incidence. At normal incidence, r is defined in terms of the index of refraction n and the extinction coefficient k as

$$r = \frac{n - ik - 1}{n - ik + 1} \quad (\text{Ref 14}) \quad (2)$$

Equating Equations 1 and 2 at normal incidence, we arrive at

$$n = \frac{1 - R}{1 + R - 2\sqrt{R} \cos \varphi} \quad (3)$$

and

$$k = \frac{2\sqrt{R} \sin \varphi}{1 + R - 2\sqrt{R} \cos \varphi} \quad (4)$$

Other pertinent relations are

$$\epsilon = \epsilon_1 - i\epsilon_2 = (n - ik)^2 \quad (5)$$

$$\epsilon_1 = n^2 - k^2 \quad (6)$$

$$\epsilon_2 = 2nk \quad (7)$$

and

$$\alpha = \frac{4\pi k}{\lambda} \quad (8)$$

where ϵ is complex dielectric constant, α the absorption coefficient, and λ the wavelength.

The natural logarithm of Equation 1 is

$$\ln r = \frac{1}{2} \ln R - i\psi \quad (9)$$

The imaginary part of Equation 9 may now be written as an integral transform of the measured reflectivity by using the Kramers-Kronig relation¹²

$$\psi_0 = -\frac{E_0}{\pi} \int_0^\infty \frac{\ln R}{E^2 - E_0^2} dE \quad (10)$$

where E is the energy of the incident radiation. Hence, a measurement of the reflectivity over the entire energy spectrum enables one to calculate the phase angle ψ_0 and the optical constants at an arbitrary output energy E_0 .

In general, one cannot make reflectivity measurements over an infinite energy interval, for experimental difficulties appear at both low and high energies. In the soft X-ray region the reflectivity becomes quite small and must be extrapolated. The output energy E_0 should be far removed from both the high and low experimental limits, so that the contributions beyond these energies to ψ_0 are negligible.

Reflectivity measurements on metals¹⁵ and semiconductors¹⁶ have been carried out from approximately 0.001 to 25 e.v.

In order to treat the singularity of Equation 10 at $E = E_0$, we shall work with the equivalent Kramers-Kronig relation¹²

$$\varphi_0 = \frac{E_0}{\pi} \int_0^{\infty} \frac{\ln \frac{R_0}{R}}{E^2 - E_0^2} dE \quad (11)$$

where R_0 is the reflectivity at E_0 . The equality between Equations 10 and 11 immediately follows since

$$\int_0^{\infty} \frac{1}{E^2 - E_0^2} dE = 0$$

and R_0 is treated as a constant in the integration. For the construction of the computer program it is convenient to divide the contributions to φ_0 into different regions of the energy spectrum. Equation 10 will be split into four parts and integrated over three intervals, the low energy extrapolation (0 to a), the measured region (a to b), and the high energy extrapolation (b to ∞). Hence,

$$\varphi_0 = \varphi_1 + \varphi_2 + \varphi_3 + \varphi_4 \quad (12)$$

where

$$\varphi_1 = \frac{E_0}{\pi} \int_a^b \frac{\ln \frac{R_0}{R}}{E^2 - E_0^2} dE \quad (13)$$

$$\begin{aligned} \varphi_2 = \frac{E_0}{\pi} \ln R_0 \left[\int_0^a \frac{dE}{E^2 - E_0^2} + \int_b^{\infty} \frac{dE}{E^2 - E_0^2} \right] = \\ \frac{1}{2\pi} \ln R_0 \ln \left[\frac{(E_0 - a)(b + E_0)}{(E_0 + a)(b - E_0)} \right], \end{aligned} \quad (14)$$

$$\varphi_3 = -\frac{E_0}{\pi} \int_0^a \frac{\ln R}{E^2 - E_0^2} dE, \quad (15)$$

$$\varphi_4 = -\frac{E_0}{\pi} \int_b^\infty \frac{\ln R}{E^2 - E_0^2} dE. \quad (16)$$

The integral φ_1 over the measured region is evaluated numerically on the computer by Simpson's rule

$$\varphi_1 = \frac{E_0}{\pi} \int_a^b \frac{\ln \frac{R_0}{R}}{E^2 - E_0^2} dE = \frac{E_0}{\pi} \left(\frac{\Delta E}{3} \right) \left[(Y_1 + 4(Y_2 + Y_4 + Y_6 + \dots Y_{N-1}) + 2(Y_3 + Y_5 + Y_7 + \dots Y_{N-2}) + Y_N) \right], \quad (17)$$

where Y_i is the value of the integral at the i^{th} point from the lower limit of integration and ΔE is the increment of E . Simpson's rule necessitates that the energy increments be equally spaced and that the number of points N be an odd integer.

At the singularity point $E = E_0$, $R = R_0$, the integrand becomes indeterminate. By the application of L'Hospital's rule, the singularity may be evaluated in the limit as

$$\lim_{E \rightarrow E_0} Y_k = \lim_{E \rightarrow E_0} \left(\frac{\frac{d}{dE} \ln \left(\frac{R_0}{R} \right)}{\frac{d}{dE} (E^2 - E_0^2)} \right) = -\frac{1}{2E_0 R_0} \left(\frac{dR}{dE} \right)_{E=E_0} \quad (18)$$

The derivative $\left(\frac{dR}{dE} \right)_{E=E_0}$ is obtained by the approximation for numerical differentiation after smoothing¹⁷

$$\left(\frac{dR}{dE}\right)_{E=E_0} = \frac{1}{12 \Delta E} \left[(R_{K-2} - R_{K+2}) - 8(R_{K-1} - R_{K+1}) \right] \quad (19)$$

The singularity point for a test reflectivity function was found to lie on a smooth curve with the neighboring values of the integrand in Equation 17 and was included in the Simpson summation.

By inspecting the sign of the integrand in Equation 13, one can tell which parts of the energy reflectivity spectrum give a positive or negative contribution to the output phase angle. The same is true for Equation 14. φ_2 is positive when $E_0^2 < ab$ and negative when $E_0^2 > ab$ since $\ln R_0 \leq 0$ as $R \leq 1$.

The reflectivity in the extrapolated infra-red interval $(0, a)$ is constant to a high degree of approximation; thus it may be taken out of the integration. Equation 15 then reduces to

$$\varphi_3 = \frac{1}{2\pi} \ln R_a \ln \left(\frac{a + E_0}{E_0 - a} \right), \quad (20)$$

where R_a is the long wavelength value. φ_3 gives a negative contribution to the total phase angle.

The high energy extrapolation in many cases makes a significant contribution to the phase angle. One usually chooses an extrapolation such that the values of the computed optical constants agree with those obtained from direct measurements in the visible and the near ultra-violet frequency range.¹⁵ For simplicity we choose the reflectivity in the expression φ_4 to be a constant, R_c . Three different values of R_c are provided in this program. After integrating, Equation 16 becomes

$$\varphi_4 = - \frac{1}{2\pi} \ln R_c \ln \left(\frac{b + E_0}{b - E_0} \right) \quad (21)$$

and is always positive.

The choice of a constant cut-off reflectivity R_c is valid at sufficiently high energies, provided the range of integration for ϕ_1 is large. In some cases it may be necessary to put extrapolated values in ϕ_1 to get agreement with values of the optical constants measured by direct techniques. For this particular program and machine, the dimensionality of the input is 500 for the ϕ_1 integration (actually, 499 input points are available since N must be an odd integer).¹⁸ The energy input points are not entered as data but are generated by the program. The starting point corresponds to E_1 inputted as W_A , with δ as the increment. It has already been noted that energy increment must remain the same.

The output points must be appropriately chosen input points and must be equally spaced. However, the output energy increment need not be the same as the input increment. The lowest output energy values is E_3 . The other output values are determined by choosing a desired increment ($k = 1, 2, 3, \dots$).

For example, k - corresponding output points

$$1 \quad E_3, E_4, E_5 \dots E_{N-2}$$

$$2 \quad E_3, E_5, E_7 \dots$$

$$3 \quad E_3, E_6, E_9 \dots$$

$$i \quad E_3, E_{3+i}, E_{3+2i} \dots$$

The upper limit of the output points is not greater than E_{N-2} , and the lower limit is not less than E_3 . These limits are due to the evaluation of the output points near the upper and lower limits of the Simpson summation. The maximum number of output points is 495 and corresponds to the case in which there are 499 input points and $k = 1$.

THE COMPUTER PROGRAM

The Kramers-Kronig transformation was programmed for the Univac Solid State 90 computer, using Fortran II language, version 9000. The following substitutions were made as a convenience of programming:

$$\text{PHI} = \varphi$$

$$\text{RHO} = \rho$$

$$\text{RI} = R, R_0$$

$$\rho_1 = \varphi_1 + \varphi_2$$

$$\rho_2 = \rho_1 + \varphi_3$$

$$\rho_3 = \rho_2 + \varphi_4 \quad (1)$$

$$\rho_4 = \rho_2 + \varphi_4 \quad (2)$$

$$\rho_5 = \rho_2 + \varphi_4 \quad (3)$$

$$\text{OMEGA} = E, E_0$$

$$\text{DELTA} = \Delta E$$

$$\text{WA} = a = E_1$$

$$\text{WB} = b = E_N$$

$$\left. \begin{array}{l} \text{RC1} \\ \text{RC2} \\ \text{RC3} \end{array} \right\} = R \text{ (Assumed cutoff values at high energy)}$$

$$\text{RA} = R_a \text{ (low energy)}$$

$$\text{CN} = n$$

$$\text{CK} = k$$

$$\text{EPSN1} = \epsilon_1$$

$$\text{EPSN2} = \epsilon_2$$

$$\text{RATI} = \text{RATIO}-1 = \frac{\epsilon_2}{\epsilon_1^2 + \epsilon_2^2}$$

$$\text{RAT2} = \text{RATIO-2} = \frac{4\pi k}{\lambda}$$

$$\text{WLDO} = \lambda_0 = L$$

The values for R are punched with nine columns per word and ten words to a card in floating point. (If three or four columns make up an input word, the number of input storage locations would still remain the same.) These data values are read by one read statement and must be followed by a blank card.

Values for a, b, R_{C1} , R_{C2} , R_{C3} , delta, and R_a are punched in floating points with nine columns per word and seven words on one card. These are read by a single read statement. Integer values for N and K are on one card which is read by a single read statement.

The output program prints the following heading: E, L, R, PHI, n, k, EPSILON-1, EPSILON-2, RATIO-1, and RATIO-2 for each of the five values of RHO. After the print out for the first output point, the paper is spaced and the cycle is continued until the final output is calculated.

The computer program is as follows.

```
C      USS FORTRAN II *** VERSION 9000
      NO CARDS
C      KRAMERS KRONIG CALCULATIONS
      DIMENSION OMEGA(500),RI(500),PHI(6),RHO(5),CN(5),CK(5),EPSN1(5),EPSN2(5),
      IRAT1(5),RAT2(5)
      COMMON OMEGA,RI
      READ 13, #A, #B, #C1, #C2, #C3, DELTA, #A
      READ 14, N, K
      READ 11, (RI(I), I=1,N)
      RC1LN#LN(RC1)
      RC2LN#LN(RC2)
```

```

RCJLN#LN(RC3)
RALN#LN(RA)
DEL1#1./((12.0*DELTA)
DEL2#DELTA/3.0
GM6.2831854
SUM2Y#0.
OMEGA(1)#WA
DO 2 I#2,N
2 OMEGA(I)#OMEGA(I-1)+DELTA
PRINT 15,
NM1#N-1
DO 7 J#3,NM1,K
SUM4Y#0.
W02#OMEGA(J)**2
ROLN#LN(RI(J))
IGO1#1
IGO2#2
N1#1
N2#1
4 DO 3 I#N1,N2
X#OMEGA(I)**2-W02
A#ROLN-LN(RI(I))
Y#A/X
GO TO (33,34),IGO2
33 SUM4Y#SUM4Y+Y
IGO2#2
GO TO 3

```

```

34 SUM2Y#SUM2Y+Y
   IGO2#1
3  CONTINUE
   GO TO (8,9,10): IGO1
8  Y1#Y
   SUM2Y#0.
   N1#2
   N2#J-1
   IGO1#2
   GO TO 4
9  N1#J+1
   N2#N
   IGO1#3
   GO TO 4
10 SUM2Y#SUM2Y-Y
   Y#(-1.)/(2.0*R1(J)*OMEGA(J))*DEL1*(R1(J-2)-(8.0#R1(J-1))+(8.0#R1(J+1))-R1(
1J+2))
   JOE#J/2
   J1#2+JOE
   IF(J-J1) 17,17,18
18 SUM2Y#SUM2Y+Y
   GO TO 19
17 SUM4Y#SUM4Y+Y
19 PHI(1)#OMEGA(J)/3.1415927*DEL2*(Y1+4.0*SUM4Y+2.0*SUM2Y)
   WM#ANOMEGA(J)-#A
   WAPW#WA+OMEGA(J)
   D#LN(WMWA/WAPW)

```

```

WBPW#WB+OMEGA(J)
WBMW#WB-OMEGA(J)
E#LN(WBP#WBMW)
PHI(2)#ROLN/G*(D+E)
PHI(3)#RALN/G*LN(WAP#WMA)
H#LN(WBMW#BPW)
PHI(4)#RC1LN/G#H
PHI(5)#RC2LN/G#H
PHI(6)#RC3LN/G#H
RHO(1)#PHI(1)+PHI(2)
RHO(2)#RHO(1)+PHI(3)
RHO(3)#RHO(2)+PHI(4)
RHO(4)#RHO(2)+PHI(5)
RHO(5)#RHO(2)+PHI(6)
SIGMA#2.*SQRT(RI(J))
WLD0#1.2395E-04/OMEGA(J)
WLD01#12.566371/#LDO
DO 6 I#1,5
Z#1.+RI(J)-SIGMA*COS(RHO(I))
CN(I)#(1.0-RI(J))/Z
CK(I)#SIGMA*SIN(RHO(I))/Z
EPSN1(I)#CN(I)**2-CK(I)**2
EPSN2(I)#2.*CN(I)*CK(I)
RAT1(I)#EPSN2(I)/(EPSN1(I)**2+EPSN2(I)**2)
RAT2(I)#WLD01*CK(I)
6 CONTINUE
PRINT 12,OMEGA(J),#LDO,RI(J),(RHO(I),CN(I),CK(I),EPSN1(I),EPSN2(I),RAT1(I)

```

```

1,RAT2(1),1A1,5)
7 CONTINUE
11 FORMAT (10E9.3,/)
12 FORMAT (//F9.3,2XE11.5,F9.3,7(2XE11.5)/(3,7(2XE11.5)/))
13 FORMAT(7F6.3)
14 FORMAT(213)
15 FORMAT (6X1ME,12X1ML,8X1MR,10X3HPI,12X1HN,12X1MK,4X9HEPSILON-1,4X9HEPSILO
IN=2,6X7HRATIO-1,6X7HRATIO=2)

STOP
END

```

COMMENTS ON THE ACCURACY OF THE PROGRAM AND METHOD

The accuracy of the program was verified by putting a known test function into the computer. The tabulated input reflectivity was evaluated from the expression

$$R = e^{-E} \quad (22)$$

and φ_1 was integrated by Simpson's rule in the interval (a, b) . Suitable approximations were made for φ_3 and φ_4 so that no discontinuities in the selected output values appeared. From Equations 13 and 22, φ_1 may be directly integrated

$$\varphi_1 = \frac{E_0}{\pi} \int_a^b \frac{\ln[e^{(E-E_0)}]}{E^2 - E_0^2} dE = \frac{E_0}{\pi} \int_a^b \frac{dE}{E_0 + E} = \frac{E_0}{\pi} \ln \left(\frac{E_0 + b}{E_0 + a} \right) \quad (23)$$

The Univac computer values were in agreement with hand calculations from logarithmic tables to the third decimal place.

We also ran Ehrenreich and Phillip's reflectivity data on copper^{15,19} up to 24.4 e.v. on the computer. We obtained excellent agreement with their results for the optical constants in the regions from 0 to 10 e.v. after a suitable value of R_c was chosen for the ϕ_4 extrapolation.

The cut-off reflectivity can drastically change the values of the optical constants determined by the Kramers-Kronig program; for as R_c goes to zero, ϕ_4 approaches infinity. Since the reflectivity cannot be measured at extremely high energies, the Kramers-Kronig transformation is used in conjunction with values of the optical constants measured by direct methods. These include Drude-type variations employing polarized light,²⁰ the transmission interference filter method of Schulz,^{21,22} and a measure of the unpolarized reflectivity at four different angles.²³ The average cut-off reflectivity (more correctly, the average ϕ_4 contribution) is found by bracketing the known optical constants by successive approximations. Hence, one can give a reasonably good estimate of the optical constants in the regions beyond the energy interval covered by direct measurements, but well within the reflectivity limits.

When a material exhibits a sharp reflection edge, the input points must be closely spaced in order for the Simpson approximation to be accurate. The ϕ_1 integration will then extend throughout a limited region of the energy spectrum, and the optical constants may be evaluated only within this region. The reflection edge in silver drops from 90 percent to less than 1 percent between 3.4 and 3.8 e.v.^{7,15} If equal energy intervals are chosen every 0.02 e.v., the high energy input would be about 10.0 e.v. Free electron plasma edges which appear in the infrared for doped semiconductors are more extreme. The reflectivity of extrinsic InSB goes from 100 percent to 1 percent in an energy interval of 0.05 e.v.²⁴ In such cases it is necessary to increase the dimensionality of the input or to break up the ϕ_1 integration into two different energy intervals.

It is interesting to note that from our choice of the phase angle ϕ in Equation 1, to be physically meaningful,

$$0 \geq \phi \geq \pi. \quad (24)$$

Otherwise, the attenuating absorption coefficient $4\pi k/\lambda$ becomes negative and the transmitted light is greater than the incident beam at a given wavelength. This is immediately seen from Maxwell's equations, which give the amplitude of a wave travelling in the x direction through an absorbing medium as

$$A = A_0 \exp \left[2\pi i \frac{Et}{h} - 2\pi i \frac{Enx}{hc} - \frac{2\pi kx}{\lambda} \right]. \quad (25)$$

The sign and/or magnitude of ϕ_0 may, therefore, be used as a check to detect whether a card has been mispunched or the energy interval chosen for the numerical integration is too large.

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19. We are indebted to Dr. H. Ehrenrich for sending us tabulated values of the reflectivity and optical constants on copper and silver which were published in Reference 15.
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A COMPUTER PROGRAM FOR A KRAMERS-KRONIG TRANSFORMATION
OF THE OPTICAL REFLECTIVITY by R. J. Esposito,
F. Eckhardt, R. M. Robbins, and J. N. Brown
PA Report 564-16-1, Dec 63; 22 pp incl 599-01-004
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Relations involving the frequency-dependent optical constants give information on the electronic properties of solids. Power reflectivity measurements at normal incidence over a wide frequency region can be utilized in obtaining the optical constants by means of a general integral transformation known as the Kramers-Kronig transformation. A computer program based on this integral transformation has been constructed in Fortran II, version 3.000, language for a Washington Rand Solid State 90 computer. The program converts experimental reflectivity measurements into parameters containing the optical constants.

A brief presentation of the electronic quasi-particle and collective excitation modes is given in terms of the optical constants. A discussion of the approximations made in putting the integrals on the computer is also given. Two tests were made to check the accuracy of the program. First, a test reflectivity function, for which

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