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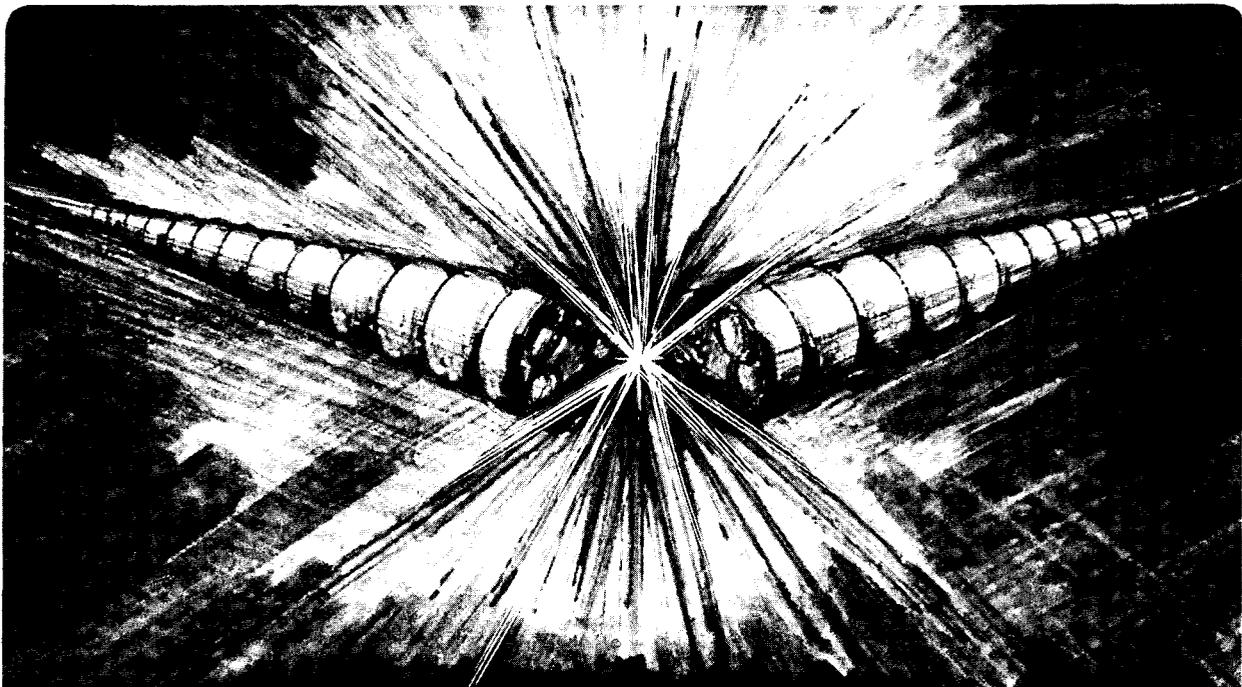
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OPTICAL SYSTEMS FOR SYNCHROTRON RADIATION:
Lecture 1. Introductory Topics

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**OPTICAL SYSTEMS FOR SYNCHROTRON RADIATION:
Lecture 1 - Introductory Topics**

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OPTICAL SYSTEMS FOR SYNCHROTRON RADIATION
(A Series of Four Lectures)

LECTURE 1:
INTRODUCTORY TOPICS

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1. INTRODUCTION

In this lecture we consider various fundamental topics which underlie the design and use of optical systems for synchrotron radiation. We choose to adopt the point of view of linear system theory which acts as a unifying concept throughout the series. In this context the important optical quantities usually appear as either impulse response functions (Green's functions) or frequency transfer functions (Fourier Transforms of the Green's functions).

2. SUMMARY OF LINEAR SYSTEM THEORY

Consider a generalised system in which an input signal $i(t)$ leads to an output signal $o(t)$. If i_1 leads to o_1 and i_2 to o_2 and if, in addition, the input ai_1+bi_2 leads to an output ao_1+bo_2 where a and b are arbitrary constants, then the system is said to be linear. The input signal $i(t) = \delta(t-t_0)$ is of special importance and the corresponding output signal $o(t) = g(t,t_0)$ is called the impulse response function or Green's Function. It should be understood as the signal at t due to a delta function input at t_0 . The impulse response function contains a full description of the properties of system.

Any arbitrary input can be synthesised from a series of delta functions and hence using the superposition principle expressed in the above

definition of linearity we can write the output quite generally as

$$o(t) = \int_{-\infty}^{+\infty} i(t_0) g(t, t_0) dt_0 \quad (1)$$

In addition to linearity many systems have the additional property that $g(t, t_0) = g(t-t_0)$ i.e. that the response to a delta function input at t_1 is the same as the response to one at t_2 apart from a shift of t_2-t_1 . For example, in a well corrected microscope the response to a point source of light in the object plane is a diffraction blur in the image plane. If the point source is shifted the diffraction blur is shifted correspondingly but retains the same shape. Such systems are called shift invariant and for these cases (1) becomes

$$o(t) = \int_{-\infty}^{+\infty} i(t_0) g(t-t_0) dt_0 \quad (2)$$

we recognise this as a convolution integral and from the Convolution Theorem we immediately have

$$O(\omega) = I(\omega).G(\omega) \quad (3)$$

Where O , I and G are the Fourier Transforms of o , i and g . For Linear, Shift Invariant Systems (3) defines the FREQUENCY TRANSFER FUNCTION $G(\omega)$ which is seen to be the Fourier Transform of the impulse response function⁸.

We have not so far given any particular physical meaning to the independant variable t . However for cases where t represents time an additional restriction applies to the system because there can be no output until after the input i.e.

$$g(t-t_0) = 0 \text{ for } t < t_0. \quad (4)$$

Such systems are called causal and we shall see later that the restriction (4) leads to the requirement that the real and imaginary parts of $G(\omega)$ form a Hilbert Transform pair.

We now consider two examples of Linear Shift Invariant Systems which are relevant to optical system design.

3. DAMPED HARMONIC OSCILLATOR

Consider an electron bound so that its natural oscillation frequency is ω_0 and lightly damped with with damping constant Γ . The impulse response function is the response to a forcing function $-eE \delta(t)$ i.e. the solution¹ to the equation.

$$m \frac{d^2 \underline{r}}{dt^2} + m\Gamma \frac{d\underline{r}}{dt} + m\omega_0^2 \underline{r} = -e\underline{E} \delta(t). \quad (5)$$

In view of the non-zero inertia of the system we need a sine solution:

$$\underline{r}(t) \equiv \underline{g}(t) = \frac{-e\underline{E}}{m\omega_0} e^{-\frac{\Gamma}{2} t} \sin \omega_0 t \quad (6)$$

By taking the Fourier Transform we arrive at the Frequency Transfer Function

$$G(\omega) = \frac{-e\underline{E}}{m} \frac{1}{\omega_0^2 - \omega^2 + i\omega\Gamma} \quad (7)$$

\underline{E} now represents the amplitude of a sine wave input to the system.

4. FREE SPACE PROPAGATION OF AN OPTICAL FIELD

Suppose we know the amplitude distribution of a wave over some plane surface Σ of finite area and general point $P(x', y')$ and we wish to find the amplitude distribution over another plane surface parallel to Σ , distance z downstream from it and having general point $Q(x, y)$. According to the Rayleigh - Sommerfeld diffraction formula²

$$U_Q(x, y) = \frac{1}{i\lambda} \int_{\Sigma} U_P(x', y') \frac{\exp ikr}{r} \cos\theta \, dx' dy' \quad (8)$$

where $PQ \equiv r$, $k = \frac{2\pi}{\lambda}$ and θ is the angle between PQ and the normal to Σ . We recognise that (8) is a linear superposition integral like (1). To simplify (8) we approximate $\cos\theta \approx 1$ and $r \approx z$ in the denominator. In the exponent we approximate

$$r = z^2 + (x-x')^2 + (y-y')^2 \approx z \left[1 + \frac{1}{2} \left(\frac{x-x'}{z} \right)^2 + \frac{1}{2} \left(\frac{y-y'}{z} \right)^2 + \dots \right] \quad (9)$$

With these simplifications which are variously known as the Fresnel, Gaussian or Paraxial approximation (8) becomes

$$U_Q(x, y) = \frac{e^{ikz}}{i\lambda z} \int_{\Sigma} U_P(x', y') \exp \frac{i\pi}{\lambda z} \left[(x-x')^2 + (y-y')^2 \right] dx' dy' \quad (10)$$

We note that (10) is now a convolution integral (like (2)) and can finally be written, using $*$ to represent convolution as

$$U_Q(x, y) = \frac{e^{ikz}}{i\lambda z} U_P(x, y) * \psi(x, y; z) \quad (11)$$

where

$$\psi(x, y; z) \equiv \psi(\underline{x}; z) = \exp \frac{i\pi \underline{x}^2}{\lambda z} \quad (12)$$

and $\underline{x} = \underline{i}x + \underline{j}y$.

The function $\psi(\underline{x}; z)$ is known as an Optical Propagator or Vander Lugt Function. These functions provide a convenient shorthand for problems

in Fourier Optics and an extensive algebra has been worked out for them³.

5. OPTICAL PROPERTIES OF MATERIALS: ELECTROMAGNETIC THEORY

Let us take as a starting point the exact form of Maxwells equations as stated for example by Born and Wolf⁴. We now make the following additional assumptions about the properties of the material we are considering:

$$\underline{j} = \sigma \underline{E} \quad \text{Ohms law} \quad (13a)$$

$$\underline{j}_{\text{ext}} = \rho_{\text{ext}} = 0 \quad \text{no external currents or charges} \quad (13b)$$

$$\underline{P} = \chi_e \underline{E} \quad \text{no non-linear electric or} \quad (13c)$$

$$\underline{M} = \chi_m \underline{H} \quad \text{magnetic effects} \quad (13d)$$

$$\text{medium is isotropic.} \quad (13e)$$

Taking these together with the following equations⁵

$$\underline{D} = \underline{E} + 4\pi \underline{P} = \epsilon \underline{E} \quad (14)$$

$$\underline{B} = \underline{H} + 4\pi \underline{M} = \mu \underline{H} \quad (15)$$

We have

$$\epsilon = 1 + 4\pi \chi_e \quad (16)$$

$$\mu = 1 + 4\pi \chi_m \quad (17)$$

χ_e and χ_m are the macroscopic electric and magnetic susceptibilities respectively. Otherwise the notation is standard as in references 4, 5 and 6. Using (13a), (13b), (14) and (15), Maxwells equations reduce to a single wave equation⁶:

$$\nabla^2 \underline{E} = \frac{\epsilon \mu}{c^2} \frac{\partial^2 \underline{E}}{\partial t^2} + \frac{4\pi \sigma}{c^2} \frac{\partial \underline{E}}{\partial t} \quad (18)$$

If we now assume²⁶ a time dependance $e^{i\omega t}$ i.e. $\partial/\partial t \equiv i\omega$ then we get the space dependant equation

$$\nabla^2 \underline{E} + \frac{\omega^2 \mu^2}{c^2} \left(\epsilon - i \frac{4\pi \sigma}{\omega} \right) \underline{E} = 0 \quad (19)$$

indicating a simple harmonic plane wave with complex propagation

constant \tilde{k} given by

$$\tilde{k}^2 = k_0^2 \mu \left(\epsilon - i \frac{4\pi \sigma}{\omega} \right) \quad (20)$$

where ω is the angular frequency and $k_0 = \frac{\omega}{c}$. Since $\tilde{k} = \tilde{n} k_0$ where $\tilde{n} = n - ik$ is the complex refractive index of the material, we can write²⁶ for non magnetic materials ($\mu=1$)

$$(n-ik)^2 = \tilde{n}^2 = \epsilon - i \frac{4\pi \sigma}{\omega} \quad (21)$$

so that

$$n^2 - k^2 = \epsilon, \quad 2nk = \frac{4\pi\sigma}{\omega} \quad (22)$$

Alternatively we can represent the last term in (21) as the imaginary part of a complex dielectric function $\tilde{\epsilon} = \epsilon_1 - i\epsilon_2$ where

$$\epsilon_1 = \epsilon, \quad \epsilon_2 = \frac{4\pi\sigma}{\omega} \quad (23)$$

Another common notation is $\tilde{n} = 1 - \delta - i\beta$. In all cases the real part represents dispersion; changes in phase velocity, wavelength etc. compared to vacuum. The imaginary part represents absorption. The plane wave solution to (19) thus becomes²⁵

$$\underline{E} = \underline{E}_0 \exp-i[\underline{n}\underline{k}_0 \cdot \underline{r} - \omega t] \exp-k\underline{k}_0 \cdot \underline{r} \quad (24)$$

The linear absorption coefficient μ is given by

$$\mu = 2kk_0 = \frac{4\pi k}{\lambda} \quad (25)$$

In considering these optical constants it is important to note that for $\lambda > 100$ eV, $|1-n| \equiv |\delta| \ll 1$ and $k \equiv \beta \ll 1$.

6. THEORY OF DISPERSION

Initially let us represent an electron in an atom as a damped harmonic oscillator with a single natural frequency as in equations (5) - (7). Then we can see that we have an atomic dipole moment $\underline{p} = -e\underline{r} = \tilde{\alpha}\underline{E}$.

The complex atomic polarisability $\tilde{\alpha}$ is thus from (7)

$$\tilde{\alpha} = \frac{e^2}{m} \frac{1}{\omega_0^2 - \omega^2 + i\Gamma\omega} \quad (26)$$

The macroscopic polarisation $\underline{P} = N\tilde{\alpha}\underline{E}$ where N is the number of oscillators per unit volume, so that from (13c) $\chi_e = N\tilde{\alpha}$ and from (16)

$$\tilde{\epsilon} = 1 + 4\pi N\tilde{\alpha}$$

or

$$\tilde{\epsilon}(\omega) = 1 + \frac{4\pi Ne^2}{m} \frac{1}{\omega_0^2 - \omega^2 + i\Gamma\omega} \quad (27)$$

The behavior of the dielectric function in equation (27) is shown in Fig. 1.

In order to be more realistic we need to recognize that atoms effectively contain many oscillators of different natural frequencies, each frequency corresponding to the energy of an allowed electronic transition. Suppose there are n_0 atoms per unit volume and each contains g_s oscillators of natural frequency ω_s . In this case $N = n_0 \sum g_s$ and (27) becomes

$$\tilde{\epsilon}(\omega) = 1 + \frac{4\pi n_0 e^2}{m} \sum_s \frac{g_s}{\omega_s^2 - \omega^2 + i\Gamma\omega} \quad (28)$$

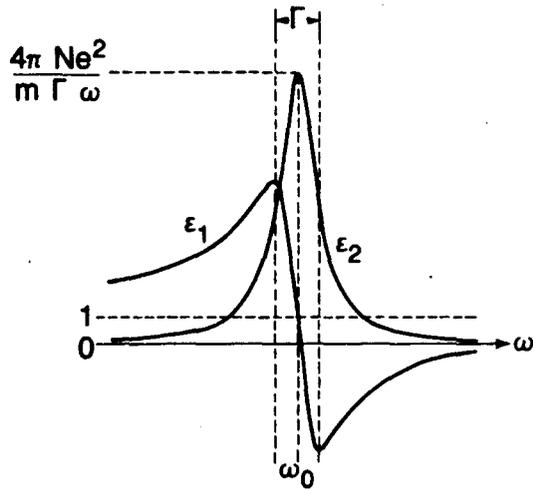
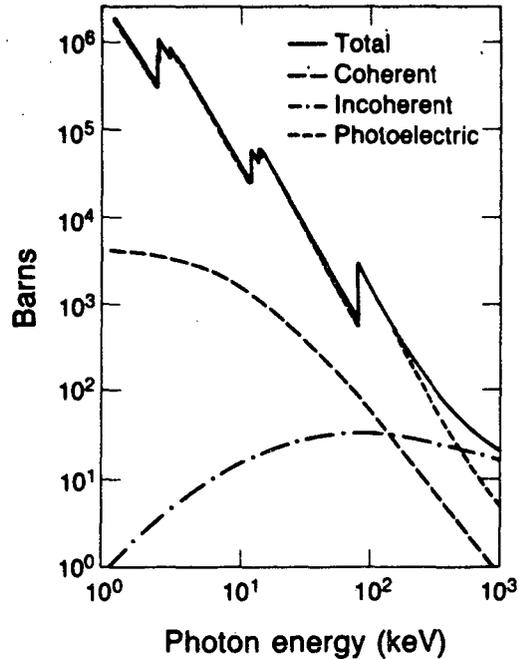
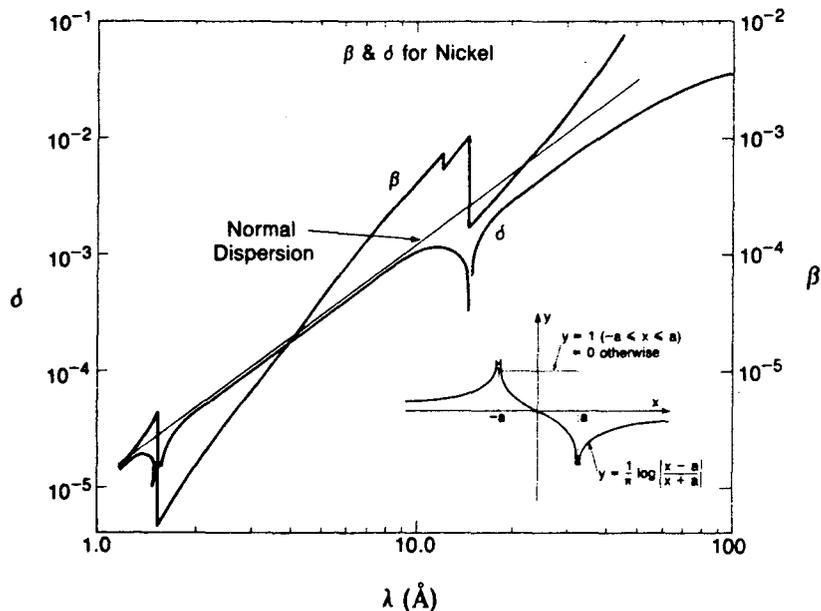


Fig 1. Behavior of the real and imaginary parts of $\epsilon = \epsilon_1 - i\epsilon_2$ for N oscillators per unit volume, each with resonant frequency ω_0 , according to equation (27)



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Fig 2. Sample x-ray cross section data from reference 12. The curves show cross sections for photoelectric absorption, coherent and incoherent scattering and the total cross section for gold. Note that in the entire region of interest here absorption is the dominant process.



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Fig 3. Values of β and δ for nickel in the range 1-100Å taken from reference 19. Notice the K edge at 8.3 keV and L edges at 0.86 keV. The inset shows a rectangular pulse and its Hilbert Transform. One can see the similarity in the effects of a step in the two cases.

In view of this derivation it becomes clear that $\tilde{\epsilon}(\omega)-1$ is the frequency transfer function for the material as the linear system, with $\underline{E}(\omega)$ as input and $\underline{P}(\omega)$ as output.

From (27) we can see the limiting behavior of $\tilde{\epsilon}(\omega)$ for $\omega \gg \omega_0$ i.e. electron binding forces negligible:

$$\lim_{\omega \rightarrow \infty} [\tilde{\epsilon}(\omega)] = 1 - \frac{\omega_p^2}{\omega^2} \quad (29)$$

where $\omega_p^2 = \frac{4\pi Ne^2}{m}$ and ω_p is known as the plasma frequency

This description represents a crude model for dealing with free electrons and it has relevance in describing the interaction of low energy photons with conduction electrons. In this case it is known as the Drude model. It is also important as the asymptotic form of $\tilde{\epsilon}(\omega)$ for deriving sum rules²⁰.

Ultimately the most important property of our oscillators is their strength as scatterers of an incoming wave. To calculate this we first observe that an incoming transverse electromagnetic wave creates an oscillating dipole whose dipole moment is perpendicular to the wave propagation direction (the axis, say) and has dipole moment $\tilde{\alpha}\underline{E}$ which is given by (26). The field at an axial point distant r from the dipole is \underline{E}_p where⁷.

$$\underline{E}_p = \frac{\omega^2 \underline{E}(t-\frac{r}{c})}{c^2 r}$$

substituting for $\underline{p}(\tilde{\alpha}\underline{E})$ from (26) we get for our oscillator

$$\underline{E}_p = \frac{e^2}{mc^2 r} \frac{\omega^2 \underline{E}(t-\frac{r}{c})}{\omega_s^2 - \omega^2 + i\Gamma\omega} \quad (30)$$

Suppose now the electron oscillator were to become a free electron. This would be achieved by setting $\omega_s \rightarrow 0$, $\Gamma \rightarrow 0$. Then (30) would become

$$\underline{E}_p' = \frac{e^2}{mc^2 r} \underline{E}(t-\frac{r}{c}) \quad (31)$$

We can now calculate the scattering strength of our oscillator relative to a free electron. This quantity is known as the SCATTERING FACTOR of the oscillator f_s . From (29) and (30) $f_s = \underline{E}_p / \underline{E}_p'$ or

$$f_s = \frac{-\omega^2}{\omega_s^2 - \omega^2 + i\omega\Gamma} \quad (32)$$

Now using $c = \omega\lambda/2\pi$ and the classical electron radius r_0 given by $r_0 = e^2/mc^2$ (28) becomes

$$\tilde{\epsilon}(\omega) = 1 - \frac{n_0 r_0 \lambda^2}{\pi} \sum_S \epsilon_S f_S \quad (33)$$

Apparently the quantity $\sum_S \epsilon_S f_S$ is an intrinsic property of an atom. It is called the atomic scattering factor and is usually written as $f=f_1+if_2$. Substituting this in (33) we have

$$\tilde{\epsilon}(\omega) = 1 - \frac{n_0 r_0 \lambda^2}{\pi} (f_1 + if_2) \quad (34)$$

and using (22) and (23) with $1-n=\delta$ and $k=\beta$ both small we finally get

$$\delta = \frac{r_0 n_0}{2\pi} \lambda^2 f_1 = A \lambda^2 f_1 \quad (35)$$

$$\beta = \frac{r_0 n_0}{2\pi} \lambda^2 f_2 = A \lambda^2 f_2 \quad (36)$$

where $A = 2.72 \times 10^{-6} \frac{\rho}{M} \text{ \AA}^{-2}$, $r_0 = 2.818 \times 10^{-13} \text{ cm}$, and ρ is the density in gm/cm^3 and M the atomic weight.

A knowledge of f_1 and f_2 or their equivalents is extremely important in designing optical systems and there are extensive tabulations in the literature. Because of its direct relationship to the absorption coefficient and the absorption cross-section σ , f_2 is easier to measure and is more widely known and tabulated than f_1 . For reference we recall that the linear absorption coefficient is given by

$$\mu = \frac{4\pi\beta}{\lambda} = 2r_0 \lambda n_0 f_2 = n_0 \sigma \quad (37)$$

In the next section we show that since $\tilde{\epsilon}(\omega)$ is a frequency transfer function of a casual system, its real and imaginary parts must form a Hilbert Transform pair. Anticipating this result we find¹⁴

$$\delta(\omega) = A \lambda^2 \left[Z + \frac{1}{\pi^2 r_0 c^2} \int_{-\infty}^{+\infty} \frac{\beta(\omega') \omega' d\omega'}{\omega^2 - \omega'^2} \right] \quad (38)$$

This is the relation usually used to derive δ or f_1 values from a set of measurements of β or f_2 . (38) has two terms the first or "normal dispersion" term, which describes the dispersion for an atom comprising Z free electrons and the second or "anomalous dispersion" term which describes the response of the resonant system consisting of the oscillators. The second term becomes negligible for frequencies much larger than the largest resonant frequency.

We show in table I a survey of the main compilations of optical constants data for both VUV and x-ray energies. In figures 2, 3 and 4

we show typical data from such sources. In using these data we offer various points to be noted :

(i) Unique values of f_1 and f_2 only exist for photon wavelengths somewhat larger than the atomic size. For shorter wavelengths the useful quantity for us is the scattering factor near the forward direction.

(ii) The above theory was written with photon energies above 100eV in mind. In this case the allowed transitions having significant g_s values in (28) are essentially from atomic bound states into the continuum. This is not a necessary restriction and transitions dominated by solid state effects, interband, intraband etc can be included without changing the formalism except that δ and β ($1-n$ and k) may no longer be small.

(iii) Tabulations above 100eV depend on measurements or calculations that are specifically atomic in character. They do not include anything to account for solid state effects such as EXAFS, XANES etc. Generally speaking they also make no attempt to follow the functions when they are rapidly varying near absorption edges. Behavior in these regions is usually approximated as a sharp step.

(iv) Significant disagreements among the various sources and between theory and experiment are quite common. Efforts continue to improve this situation. The following³² gives an idea of the accuracy with which optical constants are known:

Below 1 keV	30-50% inconsistencies among theories, sparse experimental data
1-5 keV	Sources agree within 5-10%, occasionally 20%
Above 5 keV	Sources agree within 2-5% except within 10% above threshold when variations are 10% for low Z, 5-10% for high Z.

(v) In some wavelength ranges f_1 values are hard to find. To get f_1 values in these ranges one can either apply equation (38) or utilize the universal dispersion curves provided by Parratt and Hempstead¹⁰. Either way considerable effort is involved.

(vi) Optical constants of compounds and mixtures can be calculated by taking the weighted averages of the elemental constituents. This procedure is obviously good only when atomic effects dominate.

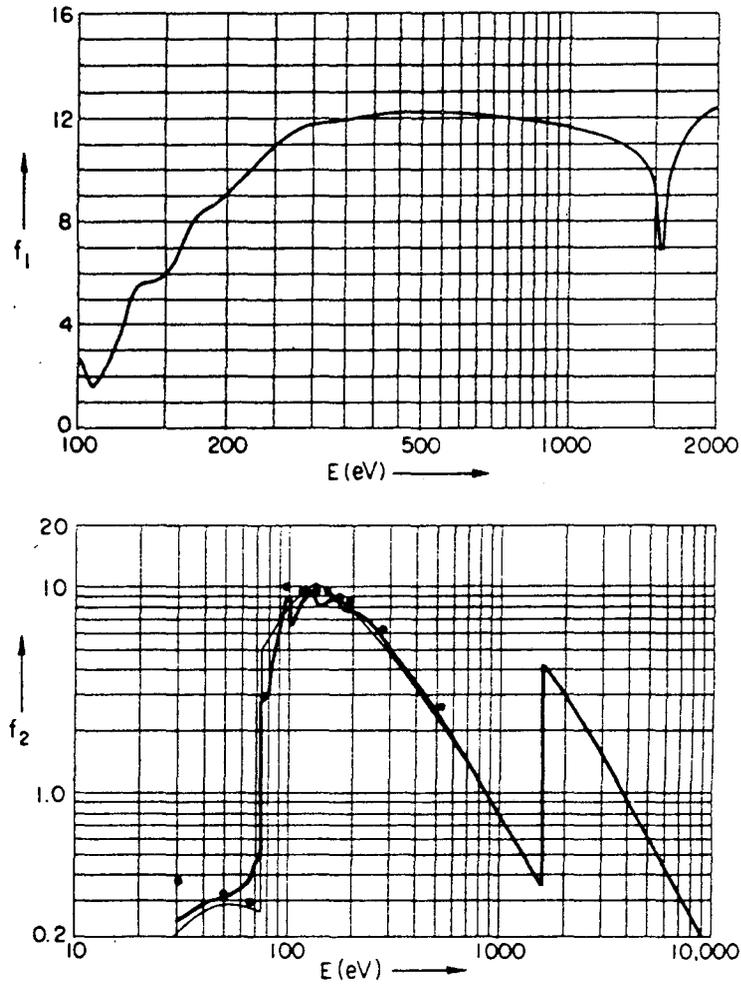
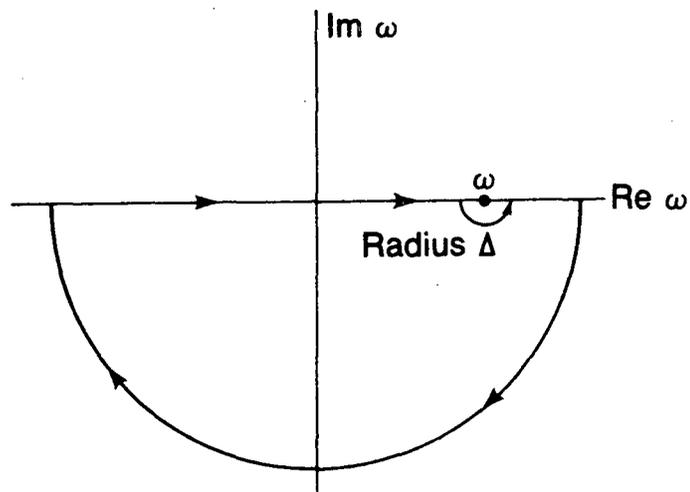


Fig 4. A sample from the tabulation of Henke *et al.* (reference 14 (ii)) showing f_1 and f_2 values for aluminium.



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Fig 5. The contour c used in equation (41)

7. KRAMERS KRONIG RELATIONS

Since $\tilde{\epsilon}(\omega)-1$ is a frequency transfer function there must be a causal, shift invariant impulse response function $g(t-t_0)$, so that

$$\tilde{\epsilon}(\omega)-1 = \int_{-\infty}^{+\infty} g(\tau)e^{-2\pi i\omega\tau}d\tau \quad (39)$$

where $\tau = t-t_0$ and $g(\tau) = 0$ for $\tau < 0$. Suppose for the moment that $\omega = \omega_1+i\omega_2$. (39) then becomes

$$\tilde{\epsilon}(\omega)-1 = \int_{-\infty}^{+\infty} g(\tau)e^{-2\pi i\omega_1\tau} e^{-2\pi\omega_2\tau} d\tau \quad (40)$$

It is apparent from the last term of the integrand in (40) that for $\tau > 0$. The integral remains bounded only if $\omega_2 < 0$. Thus

$\tilde{\epsilon}(\omega)-1$ is analytic only in the lower half plane. We also consider that $\tilde{\epsilon}(\omega)-1 \rightarrow 0$ as $|\omega| \rightarrow \infty$. This is because $\tilde{\epsilon}(\omega)-1$ represents a physical property of a material and no material is elastic enough to respond to an input at infinite frequency.

With these understandings the integral

$$I = \int_c \frac{\tilde{\epsilon}(\omega')-1}{\omega'-\omega} d\omega' \quad (41)$$

(with the contour c shown in fig 5) must, by Cauchy's Theorem⁹, be equal to zero. Defining integrals that go clockwise round the contour as positive we get

$$I = I_{\text{large circle}} + I_{\text{real axis}} - \frac{1}{2} I_{\text{small circle}} \quad (42)$$

or substituting values

$$0 = 0 + \int_{-\infty}^{\omega'-\Delta} + \int_{\omega'+\Delta}^{+\infty} - \frac{1}{2} \cdot 2\pi i \{ \tilde{\epsilon}(\omega)-1 \} \quad (43)$$

where the value of the last term follows from Cauchy's integral formula⁹. Taking the limit of (43) as $\Delta \rightarrow 0$ we get the result

$$\tilde{\epsilon}(\omega)-1 = \frac{1}{i\pi} P \int_{-\infty}^{+\infty} \frac{\epsilon(\omega')-1}{\omega'-\omega} d\omega', \quad (44)$$

where P indicates the Cauchy principle value. Taking real and imaginary parts of (44) with $\tilde{\epsilon} = \epsilon_1 - i\epsilon_2$

$$\epsilon_1(\omega)-1 = - \frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{\epsilon_2(\omega')}{\omega'-\omega} d\omega' \quad (45)$$

and
$$\epsilon_2(\omega) = \frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{\epsilon_1(\omega')-1}{\omega'-\omega} d\omega' \quad (46)$$

The signs of (45) and (46) would be reversed²⁵ for $\tilde{\epsilon} = \epsilon_1 + i\epsilon_2$. (45) and (46) are a form of the Kramers-Kronig²³ relations for $\tilde{\epsilon}(\omega)-1$ and indicate that the real and imaginary parts of $\tilde{\epsilon}(\omega)-1$ indeed form a Hilbert Transform pair²⁴. The same proof is applicable to any causal frequency transfer function. It is usual to apply certain arguments²⁷ and rewrite (45) and (46) as

$$\epsilon_1(\omega)-1 = -\frac{2}{\pi} P \int_0^{\infty} \frac{\epsilon_2(\omega')\omega'}{\omega'^2-\omega^2} d\omega' \quad (47)$$

$$\epsilon_2(\omega) = -\frac{4\pi\sigma(0)}{\omega} + \frac{2\omega}{\pi} \int_0^{\infty} \frac{\epsilon_1(\omega')-1}{\omega'^2-\omega^2} d\omega' \quad (48)$$

where $\sigma(0)$ is the d.c. conductivity.

It is not possible to identify the refractive index directly as a frequency transfer function, however we can still get Kramers Kronig relations for it by the following argument²⁸. $\tilde{n}(\omega)$ is analytic in the lower half plane since $\tilde{n}^2 = \tilde{\epsilon}$ and an analytic function of an analytic function must be another analytic function. Thus the main argument for $\tilde{\epsilon}(\omega)-1$ can be used for $\tilde{n}(\omega)-1$ and (47) and (48) can be shown to become²⁸

$$n(\omega)-1 = -\frac{2}{\pi} P \int_0^{\infty} \frac{k(\omega')\omega'}{\omega'^2-\omega^2} d\omega' \quad (49)$$

$$k(\omega) = \frac{2\omega}{\pi} P \int_0^{\infty} \frac{n(\omega')-1}{\omega'^2-\omega^2} d\omega' \quad (50)$$

Useful dispersion relations for many other quantities for example the amplitude reflectance⁶ can be worked out and are important for analysing optical data. Reviews can be found in references 6, 20 and 28.

There are further restrictions on the form of the optical constants which can be traced to the fact that all physical systems have some inertia and so their impulse response functions must be zero at time zero. Such restrictions are called inertial sum rules and are reviewed in reference 20. The best known sum rule is the "f-sum rule" and we can derive it easily by considering the high frequency behavior of, for example, $n(\omega)$. Equating the square root of (29) to the high frequency limit of (49) we immediately get

$$\int_0^{\infty} \omega k(\omega) d\omega = \frac{\pi}{4} \omega_p^2 \quad (51)$$

In view of (39) it is not surprising that the $t \rightarrow 0$ behavior of $n(\omega)-1$ can be studied by considering $\omega \rightarrow \infty$.

TABLE 1

<u>Author</u>	<u>Ref.</u>	<u>Materials</u>	<u>Constants</u>	<u>Energies</u>	<u>Grid spacing</u>
McMaster <u>et al.</u>	11	all elements	absorption cross sections	10^3-10^6 eV	10-20%
Plechaty <u>et al.</u>	12	all elements	only ditto	10^2-10^8 eV	10-20%
Veigele	13	all elements	ditto	10^2-10^8 eV	10-20%
Henke <u>et al.</u> (i)	14	all elements	f_1 & f_2	100-2000eV*	~2.5%
Henke <u>et al.</u> (ii)		all elements	f_1 & f_2	100-2000eV(f_1) 30-10000eV(f_2)	~10% (lines)
Kirz <u>et al.</u> steps	15	Elements 3,4,8...	f_1 & f_2	100-10,000eV	10^2 or 10^3
Haelbich and Iwan	16	Rare gas sols alk halides	μ	~5-5000eV (variable)	graphs only
Weaver <u>et al.</u>	17	Most metals	$\epsilon_1 \epsilon_2 n k$ $Im(\frac{1}{\epsilon})$ normal R	~.1-30eV (variable)	.05eV
Hageman <u>et al.</u>	18	Mg Al Cu Ag Au Bi C Al ₂ O ₃	ditto plus N_{eff}	~.01-5x10 ⁴ eV	10-50%
Zombeck and Austin	19	Ni,Au,Pt,	n, k grazing R	100-10,000eV	10%
Palik (ed)	20	11 metals, 14 semi cons, 12 insulators	n, k	IR-2000eV as appropriate	various
Sasaki**	21	all elements	f_1 & f_2	.1-2.89Å	.01Å
Hettrick	22	Ni,Au,Ru,Pt, Ir,Rh,Os,Re,W	n, k grazing R	100-10,000eV	10% & graphs
Auerbach and Tirsell	29	all elements	f_1 & f_2	100-10,000eV	graphs & digital storage
Henke and Schattenburg	30	elements 1-32	μ	100-1500eV	parameter fits
Biggs and Lighthill	31	all elements	absorption cross-sections	10^1-10^6 eV	parameter fits

* data up to 10,000eV on digital storage

**computed values using Cromer and Liberman code

REFERENCES

1. E. Butkov, "Mathematical Physics", (Addison Wesley Reading, Mass, 1968)
2. J.W. Goodman, "Introduction to Fourier Optics", (McGraw Hill, San Francisco, 1968), p.45
3. See for example F.P. Carlson and R.E. Francis Proc. IEEE 65, 10(1977), A. Vander Lugt, Proc. IEEE 54, 8, 1055(1966)
4. M. Born and E. Wolf, "Principles of Optics", (Pergamon Press, London, 1959), pp.1 and 608
5. L.D. Landau and E.M. Lifshitz, "Electrodynamics of continuous media", (Pergamon, Oxford, 1960). pp 37, 114
6. F. Wooten, "Optical Properties of Solids", (Academic, New York, 1972). (For derivation of (18) see p26)
7. See for example R.P. Feynman, R.B. Leighton and M. Sands, "The Feynman Lectures on Physics", (Addison Wesley, Reading, Mass, 1963)
8. Note that the definitions of time dependence and of the Fourier Transform must be consistent with regard to signs. For a wave $e^{\pm i\omega t}$ one must have $G(\omega) = \int_{-\infty}^{+\infty} g(t)e^{\mp 2\pi i\omega t} dt$
9. H. Margenan, G.M. Murphy "The Mathematics of Physics and Chemistry" (Van Nostrand, Princeton 1956)
10. L.G. Parratt & C.F. Hempstead, Phys. Rev. 94, 1593(1954). W.M. McMaster, N. Kerr Del Grande, J.H. Mallett, J. H. Hubbell, UCRL-50174-Sec2-R1, Lawrence Radiation Laboratory, 1969
12. E.F. Plechaty, D.E. Cullen, R.J. Howerton UCRL-50400-Vol 6, Rev 3, Lawrence Livermore National Laboratory, 1981
13. W.J. Veigele, Atomic Data Tables 5, 51(1973)
14. (i) B.L. Henke, P. Lee, T.J. Tanaka, R.L. Shimabukuro, B.K. Fujikawa, Conf. on Low Energy X-ray Diagnostics, Monterey 1981, AIP #75,P340
(ii) B.L. Henke, P. Lee, T.J. Tanaka, R.L. Shimabukuro, B.K. Fujikawa Atomic Data and Nuclear Data Tables 27, 1(1982)
15. J. Kirz et al. (eds), "X-ray Data Booklet", Lawrence Berkeley Laboratory (PUB490), Berkeley, 1985
16. R.P. Haelbich, M. Iwan, E.E. Koch, "Optical properties of some insulators in the vacuum ultra violet region", (Physik Daten,

Fach-informations-zentrum, Karlsruhe 1977)

17. J. H. Weaver, C. Krafka, D.W. Lynch, E.E. Koch "Optical properties of metals", two volumes, (Physik Daten, Fach-informations-zentrum, Karlsruhe 1981)
18. J.H. Hageman, W. Gudat, C. Kunz, DESY SR-74/7 (1974)
19. M.V. Zombeck, Smithsonian Astrophysical Observatory report SAO-AXAF-83-016 (1980)
20. E.E. Palik (ed) "Handbook of Optical Constants of Solids", (Academic, Orlando, 1985)
21. S. Sasaki KEK 83-22 (1984)
22. M.C. Hettrick private communication
23. H.A. Kramers, Phys. Z. 30, 522(1929), R. de L. Kronig, J. Opt. Soc. Am 12, 547(1926)
24. See for example R.N. Bracewell, "The Fourier Transform and its applications", (McGraw-Hill, New York, 1978)
25. The definitions $\tilde{n}=n-ik$, $\tilde{\epsilon}=\epsilon_1-i\epsilon_2$ are consistent with the choice of sign $\underline{E}=\underline{E}_0 \exp-ik\underline{r}$ for the spatial part of a plane wave. The values of k and ϵ_2 are then positive and absorption is represented as a decaying exponential in equation (24)
26. The imaginary part of $\tilde{n}^2=\tilde{\epsilon}$ is seen to be negative for a time dependance $e^{i\omega t}$ (positive for $e^{-i\omega t}$)
27. The arguments are:
 - (i) From (23) $\tilde{\epsilon}(\omega)-1$ has a pole at $\omega=0$ if $\sigma > 0$ (which is true for metals) which we have not yet considered. We thus make another indent in the contour in fig 5 at $\omega'=0$ similar to $\omega'=\omega$ and observe that the right hand side of (43) now has an extra term $\frac{1}{2} \cdot 2\pi i \int_{c_1} \frac{-4\pi i \sigma(\omega')}{\omega'} \cdot \frac{d\omega'}{\omega'-\omega}$. where c_1 is a small circle round the origin. Using the Residue theorem (reference 1), this is $\frac{1}{2} \cdot 2\pi i (4\pi \sigma(0)/\omega)$ from which the $\sigma(0)$ term in (48) follows.
 - (ii) Since the inputs and outputs are real physical quantities, $g(\tau)$ in (39) must be real. Therefore $\tilde{\epsilon}(\omega)-1$ must be Hermitian i.e. its real part even and its imaginary part odd (reference 24). Thus $\epsilon_1(\omega)=\epsilon_1(-\omega)$ and $\epsilon_2(\omega)=-\epsilon_2(-\omega)$

(iii) Multiply the integrands in (45) and (46) by $(\omega'+\omega)/(\omega'+\omega)$ and apply (ii). (47) and (48) follow.

28. F. Bassani and M. Alterelli in "Handbook of synchrotron radiation", vol 1A, E-E. Koch (ed) (North Holland, Amsterdam, 1983)
29. J. Auerbach and G. Tirsell, UCRL report 91230 Lawrence Livermore Laboratory
30. B.L. Henke, M.L. Schattenburg, "Advances in X-ray Analysis", vol 19, p.749 (Kendall/Hunt, Iowa, 1976)
31. F. Biggs and R. Lighthill, "Analytical Approximations for X-ray cross-sections", Sandia Laboratory SC-RR-71-0507(1971)
32. N. Del Grande, Private Communication

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