1 Fundamental Optical Properties of Materials I

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1.1 INTRODUCTION

Optical properties of a material change or affect the characteristics of light passing through it by modifying its propagation vector or intensity. Two of the most important optical properties are the refractive index *n* and the extinction coefficient *K*, which are generically called *optical constants*; though some authors include other optical coefficients within this terminology. The latter is related to the attenuation or absorption coefficient α. In this chapter we present the complex refractive index, the frequency or wavelength dependence of *n* and *K*, so-called dispersion relations, how *n* and *K* are interrelated, and how *n* and *K* can be determined by studying the transmission as a function of wavelength through a thin film of the material. Physical insights into *n* and *K* are provided in Chapter 2.

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The optical properties of various materials, with n and K being the most important, are available in the literature in one form or another, either published in journals, books and handbooks or posted on websites of various researchers, organizations (e.g., NIST) or companies (e.g., Schott Glass). Nonetheless, the reader is referred to the works of Wolfe [1.1], Klocek [1.2], Palik [1.3, 1.4], Ward [1.5], Efimov [1.6], Palik and Ghosh [1.7], Nikogosyan [1.8], and Weaver and Frederikse [1.9] for the optical properties of a wide range of materials. Adachi's books on the optical constants of semiconductors are highly recommended [1.10–1.12] along with Madelung's third edition of 'Semiconductors: Data Handbook' [1.13]. There are, of course, other books and handbooks that also contain optical constants in various chapters; see, for example, references [1.14–1.17].

There are available a number of experimental techniques for measuring n and K, some of which have been summarized by Simmons and Potter [1.18]. For example, ellipsometery measures changes in the polarization of light incident on a sample to sensitively characterize surfaces and thin films. The interaction of incident polarized light with the sample causes a polarization change in the light, which may then be measured by analysing the light reflected from the sample. Recently, Collins has provided an extensive in-depth review of ellipsometery for optical measurements [1.19]. One of the most popular and convenient optical measurements involves passing a monochromatic light through a thin sample, and measuring the transmitted intensity as a function of wavelength, $T(\lambda)$, using a simple spectrophotometer. For thin samples on a thick transparent substrate, the transmission spectrum shows oscillations in $T(\lambda)$ with the wavelength due to interferences within the thin film. Swanepoel's technique uses the $T(\lambda)$ measurement to determine n and K, as described in Section 1.4.

1.2 OPTICAL CONSTANTS

One of the most important optical constants of a material is its refractive index, which in general depends on the wavelength of the electromagnetic wave, through a relationship called *dispersion*. In materials where an electromagnetic wave can lose its energy during its propagation, the refractive index becomes complex. The real part is usually the refractive index, n, and the imaginary part is called the *extinction coefficient*, K. In this section, the refractive index and extinction coefficient will be presented in detail along with some common dispersion relations. A more practical and a semiquantitative approach is taken along the lines in [1.18, 1.20, 1.21] rather than a full dedication to rigour and mathematical derivations. More analytical approaches can be found in other texts, e.g. [1.22].

1.2.1 Refractive index and extinction coefficient

The refractive index of an optical or dielectric medium, n, is the ratio of the velocity of light c in vacuum to its velocity v in the medium; $n = c/v$. Using this and Maxwell's equations, one obtains the well known Maxwell's formula for the refractive index of a substance as $n = \sqrt{\varepsilon_r \mu_r}$, where ε_r is the static dielectric constant or relative permittivity and μ_r the relative permeability. As $\mu_r = 1$ for nonmagnetic substances, one gets $n = \sqrt{\varepsilon_r}$, which is very useful in relating the dielectric properties to optical properties of materials at any particular frequency of interest. As ε_r depends on the wavelength of light, the refractive index also depends on the wavelength of light, and this dependence is called *dispersion*. In addition to dispersion, an electromagnetic wave propagating through a lossy medium experiences attenuation, which means it loses its energy, due to various loss mechanisms such as the generation of phonons (lattice waves), photogeneration, free carrier absorption, scattering, etc. In such materials, the refractive index becomes a complex function of the frequency of the light wave. The complex refractive index, denoted by n^*, with real part n, and imaginary part K, called the extinction coefficient, is related to the complex relative permittivity, $\varepsilon_r = \varepsilon_r' - j\varepsilon_r''$, by:

$$n^* = n - jK = \sqrt{\varepsilon_r} = \sqrt{\varepsilon_r' - j\varepsilon_r''} \tag{1.1a}$$

where ε_r' and ε_r'' are, respectively, the real and imaginary parts of ε_r. Equation (1.1b) gives:

$$n^2 - K^2 = \varepsilon_r' \quad \text{and} \quad 2nK = \varepsilon_r'' \tag{1.1b}$$

In explicit terms, n and K can be obtained as:

$$n = \left(1/2^{1/2}\right)\left[\left(\varepsilon_r'^2 + \varepsilon_r''^2\right)^{1/2} + \varepsilon_r'\right]^{1/2} \tag{1.2a}$$

$$K = \left(1/2^{1/2}\right)\left[\left(\varepsilon_r'^2 + \varepsilon_r''^2\right)^{1/2} - \varepsilon_r'\right]^{1/2} \tag{1.2b}$$

The optical constants n and K can be determined by measuring the reflectance from the surface of a material as a function of polarization and the angle of incidence. For normal incidence, the reflection coefficient, r, is obtained as

$$r = \frac{1 - n^*}{1 + n^*} = \frac{1 - n + jK}{1 + n - jK} \tag{1.3}$$

The reflectance R is then defined by:

$$R = |r|^2 = \left|\frac{1 - n + jK}{1 + n - jK}\right|^2 = \frac{(1-n)^2 + K^2}{(1+n)^2 + K^2} \tag{1.4}$$

Notice that whenever K is large, for example over a range of wavelengths, the absorption is strong, and the reflectance is almost unity. The light is then reflected, and any light in the medium is highly attenuated. (Typical sample calculations and applications may be found in ref. [1.20].)

Optical properties of materials are typically presented by showing the frequency dependences (dispersion relations) of either n and K or ε_r' and ε_r''. An intuitive guide to explaining dispersion in insulators is based on a single-oscillator model in which the electric field in the light induces forced dipole oscillations in the material (displaces the electron shells to oscillate about the positive nucleus) with a single resonant frequency ω_o. The frequency dependences of ε_r' and ε_r'' are then obtained as:

$$\varepsilon_r' = 1 + \frac{N_{\text{at}}}{\varepsilon_o}\alpha_e' \quad \text{and} \quad \varepsilon_r'' = 1 + \frac{N_{\text{at}}}{\varepsilon_o}\alpha_e'' \tag{1.5}$$

where N_{at} is the number of atoms per unit volume, ε_o is the vacuum permittivity, and α'_e and α''_e are the real and imaginary parts of the electronic polarizability, given respectively by:

$$\alpha'_e = \alpha_{eo}\frac{1-(\omega/\omega_o)^2}{\left[1-(\omega/\omega_o)^2\right]^2+(\gamma/\omega_o)^2(\omega/\omega_o)^2} \tag{1.6a}$$

and

$$\alpha''_e = \alpha_{eo}\frac{(\gamma/\omega_o)(\omega/\omega_o)}{\left[1-(\omega/\omega_o)^2\right]^2+(\gamma/\omega_o)^2(\omega/\omega_o)^2} \tag{1.6b}$$

where α_{eo} is the DC polarizability corresponding to $\omega = 0$ and γ is the loss coefficient that characterizes the electromagnetic (EM) wave losses within the material system. Using Equations (1.1)–(1.2) and (1.5)–(1.6), the frequency dependence of n and K can be studied. Figure 1.1(a) shows the dependence of n and K on the normalized frequency ω/ω_o for a simple single electronic dipole oscillator of resonance frequency ω_o.

It is seen that n and K peak close to $\omega = \omega_o$. If a material has a $\varepsilon''_r >> \varepsilon'_r$, then $\varepsilon_r \approx -j\varepsilon''_r$ and $n = K \approx \sqrt{\varepsilon''_r/2}$ is obtained from Equation (1.1b). Figure 1.1(b) shows the dependence of the reflectance R on the frequency. It is observed that R reaches its maximum value at a frequency slightly above $\omega = \omega_o$, and then remains high until ω reaches nearly $3\omega_o$; thus the reflectance is substantial while absorption is strong. The normal dispersion region is the frequency range below ω_o where n falls as the frequency decreases, that is, n decreases as the wavelength λ increases. The anomalous dispersion region is the frequency range above ω_o where n decreases as ω increases. Below ω_o, K is small and if $\varepsilon_{\mathrm{DC}}$ is $\varepsilon_r(0)$, then n becomes:

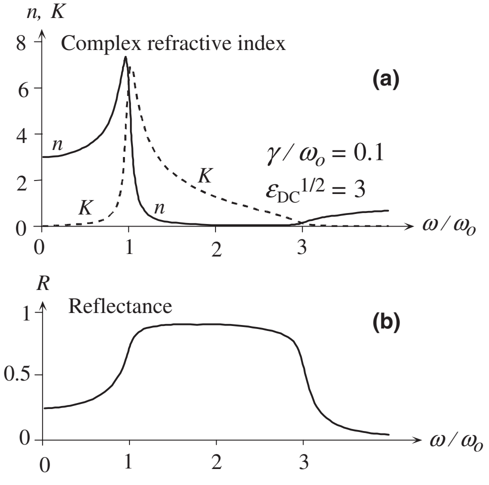

Figure 1.1 Refractive index, n and extinction coefficient K obtained from a single electronic dipole oscillator model. (a) n and K versus normalized frequency and (b) Reflectance versus normalized frequency [Reproduced from S.O. Kasap, *Principles of Electronic Materials and Devices*, 3rd Edition, McGraw-Hill, Boston, 2005]

$$n^2 \approx 1+(\varepsilon_{\text{DC}}-1)\frac{\omega_o^2}{\omega_o^2-\omega^2}; \quad \omega<\omega_o \tag{1.7}$$

Since, $\lambda = 2\pi c/\omega$, defining $\lambda_o = 2\pi c/\omega_o$ as the resonance wavelength, one gets:

$$n^2 \approx 1+(\varepsilon_{\text{DC}}-1)\frac{\lambda^2}{\lambda^2-\lambda_o^2}; \quad \lambda>\lambda_o \tag{1.8}$$

While intuitively useful, the dispersion relation in Equation (1.8) is far too simple. More rigorously, we have to consider the dipole oscillator quantum mechanically which means a photon excites the oscillator to a higher energy level, see, for example, Fox [1.21] or Simmons and Potter [1.18]. The result is that we would have a series of $\lambda^2/(\lambda^2 - \lambda_i^2)$ terms with various weighting factors A_i that add to unity, where λ_i represents different resonance wavelengths. The weighting factors A_i involve quantum mechanical matrix elements.

Figure 1.2 shows the complex relative permittivity and the complex refractive index of crystalline silicon in terms of photon energy $h\nu$. For photon energies below the bandgap energy (1.1 eV), both ε_r'' and K are negligible and n is close to 3.7. Both ε_r'' and K increase and change strongly as the photon energy becomes greater than 3 eV, far beyond the bandgap energy. Notice that both ε_r' and n peak at $h\nu \approx 3.5$ eV, which corresponds to a direct photoexcitation process, electrons excited from the valence band to the conduction band, as discussed later.

1.2.2 *n* and *K*, and Kramers–Kronig relations

If we know the frequency dependence of the real part, ε_r', of the relative permittivity of a material, then by using the Kramers–Kronig relations between the real and the imaginary

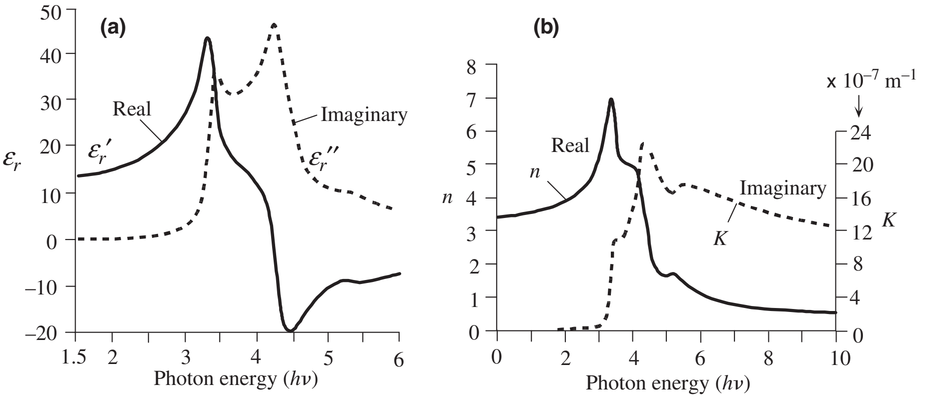

Figure 1.2 (a) Complex relative permittivity of a silicon crystal as a function of photon energy plotted in terms of real (ε_r') and imaginary (ε_r'') parts. (b) Optical properties of a silicon crystal versus photon energy in terms of real (n) and imaginary (K) parts of the complex refractive index [Data extracted from D.E. Aspnes and A.A. Studna, *Phys. Rev. B*, **27**, 985 (1983)].

parts we can determine the frequency dependence of the imaginary part ε_r'', and vice versa. The transform requires that we know the frequency dependence of either the real or imaginary part over as wide a range of frequencies as possible, ideally from zero (DC) to infinity, and that the material has linear behaviour, i.e., it has a relative permittivity that is independent of the applied field. The *Kramers–Kronig relations* for the real and imaginary parts of the relative permittivity are given by [1.23, 1.24] (see also Appendix 1C in [1.18])

$$\varepsilon_r'(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \varepsilon_r''(\omega')}{\omega'^2 - \omega^2} \mathrm{d}\omega' \tag{1.9a}$$

and

$$\varepsilon_r''(\omega) = -\frac{2\omega}{\pi} P \int_0^\infty \frac{\varepsilon_r'(\omega')}{\omega'^2 - \omega^2} \mathrm{d}\omega' \tag{1.9b}$$

where ω' is the integration variable, P represents the Cauchy principal value of the integral, and the singularity at $\omega = \omega'$ is avoided.

Similarly one can relate the real and imaginary parts of the polarizability, $\alpha'(\omega)$ and $\alpha''(\omega)$, and those of the complex refractive index, $n(\omega)$ and $K(\omega)$ as well. For $n^* = n(\omega) - jK(\omega)$,

$$n(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{K(\omega')}{\omega' - \omega} \mathrm{d}\omega' \quad \text{and} \quad K(\omega) = -\frac{2}{\pi} P \int_0^\infty \frac{K(\omega')}{\omega' - \omega} \mathrm{d}\omega' \tag{1.10}$$

It should be emphasized that the optical constants n and K have to obey what are called *f-sum rules* [1.25]. For example, the integration of $[n(\omega) - 1]$ over all frequencies must be zero, and the integration of $\omega K(\omega)$ over all frequencies gives $(\pi/2)\omega_p^2$, where $\omega_p = \hbar(4\pi NZe^2/m_e)^{1/2}$ is the free-electron plasma frequency in which N is the atomic concentration, Z is the total number of electrons per atom, and e and m_e are the charge and mass of the electron. The f-sum rules provide a consistency check and enable various constants to be interrelated.

1.3 REFRACTIVE INDEX AND DISPERSION

There are several popular models describing the spectral dependence of refractive index n in a material. Most of these are described below though some, such as the infrared refractive index, are covered under Reststrahlen absorption in Chapter 2 since it is closely related to the coupling of the EM wave to lattice vibrations. The most popular dispersion relation in optical materials is probably the Sellmeier relationship since one can sum any number of resonance-type terms to get as wide a range of wavelength dependence as possible. However, its main drawback is that it does not accurately represent the refractive index when there is a contribution arising from free carriers in narrow-bandgap or doped semiconductors.

1.3.1 Cauchy dispersion relation

In the Cauchy relationship, the dispersion relationship between the refractive index (n) and wavelength of light (λ) is commonly stated in the following form:

$$n = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} \tag{1.11}$$

where A, B, and C are material-dependent specific constants. Equation (1.11) is known as Cauchy's formula and it is typically used in the visible spectrum region for various optical glasses and is applies to *normal dispersion*, when n decreases with increasing λ [1.26, 1.27]. The third term is sometimes dropped for a simpler representation of n versus λ behaviour. The original expression was a series in terms of the wavelength, λ, or frequency, ω, or photon energy $\hbar\omega$ of light as:

$$n = a_0 + a_2\lambda^{-2} + a_4\lambda^{-4} + a_6\lambda^{-6} + \ldots \lambda > \lambda_{\text{th}} \tag{1.12a}$$

or

$$n = n_0 + n_2(\hbar\omega)^2 + n_4(\hbar\omega)^4 + n_6(\hbar\omega)^6 + \ldots \hbar\omega < \hbar\omega_{\text{tt}} \tag{1.12b}$$

where $\hbar\omega$ is the photon energy, $\hbar\omega_{\text{th}} = hc/\lambda_{\text{th}}$ is the optical excitation threshold (e.g., bandgap energy), a_0, a_2, . . . and n_0, n_2, . . . are constants. It has been found that a Cauchy relation in the following form [1.28]:

$$n = n_{-2}(\hbar\omega)^{-2} + n_0 + n_2(\hbar\omega)^2 + n_4(\hbar\omega)^4 \tag{1.13}$$

can be used satisfactorily over a wide range of photon energies. The dispersion parameters of Equation (1.13) are listed in Table 1 for a few selected materials over specific photon energy ranges.

Cauchy's dispersion relations given in Equations (1.11–1.13) were originally called the elastic-ether theory of the refractive index. It has been widely used for many materials although, in recent years, many researchers have preferred to use the Sellmeier equation described below.

1.3.2 Sellmeier dispersion equation

The Sellmeier equation is an empirical relation between the refractive index n of a substance and wavelength λ of light in the form of a series of single-dipole oscillator terms each of which has the usual $\lambda^2/(\lambda^2 - \lambda_i^2)$ dependence as in

$$n^2 = 1 + \frac{A_1\lambda^2}{\lambda^2 - \lambda_1^2} + \frac{A_2\lambda^2}{\lambda^2 - \lambda_2^2} + \frac{A_3\lambda^2}{\lambda^2 - \lambda_3^2} + \cdots \tag{1.14}$$

where λ_i is a constant, and A_1, A_2, A_3, λ_1, λ_2 and λ_3 are called *Sellmeier coefficients*, which are determined by fitting this expression to the experimental data. The actual Sellmeier

Table 1.1 Approximate Cauchy dispersion parameters of Equation (1.13) for a few materials from various sources. n_0 and n_e denote, respectively, the ordinary and extraordinary refractive indices of KDP

Material	$\hbar\omega$(eV) Min	$\hbar\omega$(eV) Max	n_{-2}(eV^2)	n_0	n_2(eV^{-2})	n_4(eV^{-4})
Diamond	0.0500	5.4700	-1.0700×10^{-5}	2.3780	0.00801	0.0001
Si	0.0020	1.08	-2.0400×10^{-8}	3.4189	0.0815	0.0125
Ge	0.0020	0.75	-1.0000×10^{-8}	4.0030	0.2200	0.1400
AlSb	0.0620	1.24	-6.1490×10^{-4}	3.1340	0.5225	0.2186
GaP	0.0571	3.60	-1.7817×10^{-3}	3.0010	0.0784	0.0058
GaAs	0.0496	2.90	-5.9737×10^{-4}	3.3270	0.0779	0.0151
InAs	0.0496	2.40	-6.1490×10^{-4}	3.4899	0.0224	0.0284
InP	0.08	3.18	-3.0745×10^{-4}	3.0704	0.1788	-0.0075
ZnSe	0.113	1.24	-4.6117×10^{-4}	2.4365	0.0316	0.0026
KDP, (n_o)	0.62	6.2	-1.7364×10^{-2}	1.5045	0.00181	0.000033
KDP, (n_e)	0.62	6.2	-4.3557×10^{-3}	1.4609	0.001859	0.000021

Table 1.2 Sellmeier coefficients of a few materials, where λ_1, λ_2, λ_3 are in µm. (From various sources and approximate values)

Material	A_1	A_2	A_3	λ_1	λ_2	λ_3
SiO_2 (fused silica)	0.696749	0.408218	0.890815	0.0690660	0.115662	9.900559
86.5%SiO_2–13.5%GeO_2	0.711040	0.451885	0.704048	0.0642700	0.129408	9.425478
GeO_2	0.80686642	0.71815848	0.85416831	0.068972606	0.15396605	11.841931
BaF_2	0.63356	0.506762	3.8261	0.057789	0.109681	46.38642
Sapphire	1.023798	1.058264	5.280792	0.0614482	0.110700	17.92656
Diamond	0.3306	4.3356		0.175	0.106	
Quartz, n_o	1.35400	0.010	0.9994	0.092612	10.700	9.8500
Quartz, n_e	1.38100	0.0100	0.9992	0.093505	11.310	9.5280
KDP, n_o	1.2540	0.0100	0.0992	0.09646	6.9777	5.9848
KDP, n_e	1.13000	0.0001	0.9999	0.09351	7.6710	12.170

formula is more complicated. It has more terms of similar form, e.g., $A_i \lambda^2/(\lambda^2 - \lambda_i^2)$, where $i = 4, 5, \ldots$, but these can generally be neglected in representing n versus λ behaviour over typical wavelengths of interest and ensuring that three terms included in Equation (1.14) correspond to the most important or relevant terms in the summation. Sellmeier coefficients for some materials as examples, including pure silica (SiO_2) and 86.5 mol.% SiO_2–13.5 mol.% GeO_2, are given in Table 2.

There are two methods for determining the refractive index of silica–germania glass $(SiO_2)_{1-x}(GeO_2)_x$: First is a simple, but approximate, linear interpolation of the refractive index between known compositions, e.g., $n(x) - n(0.135) = (x - 0.135)[n(0.135) - n(0)]/0.135$, where $n(x)$ is for $(SiO_2)_{1-x}(GeO_2)_x$; $n(0.135)$ is for 86.5 mol.% SiO_2–13.5 mol.% GeO_2; $n(0)$ is for SiO_2. Second is an interpolation for coefficients A_i and λ_i between SiO_2 and GeO_2 as reported in [1.29]:

$$n^2 - 1 = \frac{\{A_1(S) + X[A_1(G) - A_1(S)]\}\lambda^2}{\lambda^2 - \{\lambda_1(S) + X[\lambda_1(G) - \lambda_1(S)]\}^2} + \ldots \tag{1.15}$$

where X is the mole fraction of germania, S and G in parentheses refer to silica and germania, respectively. The theoretical basis of the Sellmeier equation lies in representing the solid as a sum of N lossless (frictionless) Lorentz oscillators such that each has the usual form of $\lambda^2/(\lambda^2 - \lambda_i^2)$ with different λ_i and each has different strengths, or weighting factors; A_i, $i = 1$ to N [1.30, 1.31]. Such dispersion relationships are essential in designing photonic devices such as waveguides. (Note that although A_i weight different Lorentz contributions, they do not sum to 1 since they include other parameters besides the oscillator strength f_i.) The refractive indices of most optical glasses have been extensively modelled by the Sellmeier equation. Various optical glass manufacturers such as Schott Glass normally provide the Sellmeier coefficients for their glasses [1.32]. Optical dispersion relations for glasses have been discussed by a number of authors [1.6, 1.18, 1.33]. The Sellmeier coefficients normally depend on the temperature and pressure; their dependences for optical glasses have been described by Ghosh [1.34–1.36].

There are other Sellmeier–Cauchy-like dispersion relationships that inherently take account of various contributions to the optical properties, such as the electronic and ionic polarization and interaction of photons with free electrons. For example, for many semiconductors and ionic crystals, two useful dispersion relations are:

$$n^2 = A + \frac{B\lambda^2}{\lambda^2 - C} + \frac{D\lambda^2}{\lambda^2 - E} \tag{1.16}$$

and

$$n^2 = A + \frac{B}{\lambda^2 - \lambda_o^2} + \frac{C}{(\lambda^2 - \lambda_o^2)^2} + D\lambda^2 + E\lambda^4 \tag{1.17}$$

where A, B, C, D, E, and λ_0 are constants particular to a given material. Table 3 provides a few examples. Both the Cauchy and the Sellmeier equations are strictly applicable in wavelength regions where the material is transparent, that is, the extinction coefficient is relatively small. There are many application-based articles in the literature that provide empirical dispersion relations for a variety of materials; a recent example on far-infrared substrates (Ge, Si, ZnSe, ZnS, ZnTe) is given in reference [1.37].

Table 1.3 Parameters of Equations (1.16) and (1.17) for some selected materials {Si data from D.F. Edwards and E. Ochoa, *Appl. Optics*, **19**, 4130 (1980); others from ref. [1.1]}

Material	λ_o (μm)	A	B (μm)^2	C (μm)$^{-4}$	D (μm)$^{-2}$	E (μm)$^{-4}$
Silicon	0.167	3.41983	0.159906	−0.123109	1.269×10^{-6}	-1.951×10^{-9}
MgO	0.11951	2.95636	0.021958	0	-1.0624×10^{-2}	-2.05×10^{-5}
LiF	0.16733	1.38761	0.001796	-4.1×10^{-3}	-2.3045×10^{-3}	-5.57×10^{-6}
AgCl	0.21413	4.00804	0.079009	0	-8.5111×10^{-4}	-1.976×10^{-7}

1.3.3 Refractive index of semiconductors

A. Refractive index of crystalline semiconductors

A particular interest in the case of semiconductors is in n and K for photons energies greater than the bandgap E_g for optoelectronics applications. Owing to various features and singularities in the E–$\mathbf{k}$ diagrams of crystalline semiconductors (where $\mathbf{k}$ is the electron's wave vector), the optical constants n and K for $\hbar\omega > E_g$ are not readily expressible in simple terms. Various authors, for example, Forouhi and Bloomer [1.38, 1.39], Chen et al. [1.40] have nonetheless provided useful and tractable expressions for modelling n and K in this regime. In particular, Forouhi–Bloomer (FB) equations express n and K in terms of the photon energy $\hbar\omega$ in a consistent way that obey the Kramers–Kronig relations [1.39], i.e.

$$K = \sum_{i=1}^{q} \frac{A_i(\hbar\omega - E_g)^2}{(\hbar\omega)^2 - B_i\,(\hbar\omega) + C_i} \quad \text{and} \quad n = n(\infty) + \sum_{i=1}^{q} \frac{B_{oi}(\hbar\omega) + C_{oi}}{(\hbar\omega)^2 - B_i(\hbar\omega) + C_i} \tag{1.18}$$

where q is an integer that represents the number of terms needed to suitably model experimental values of n and K, E_g is the bandgap, and A_i, B_i, C_i, B_{oi}, C_{oi} are constants, B_{oi} and C_{oi} depending on A_i, B_i, C_i, and E_g; only the latter four are independent parameters, $B_{oi} = (A_i/Q_i)[-(1/2)B_i^2 + E_gB_i - E_g^2 + C_i]$; $C_{oi} = (A_i/Q_i)[(1/2)(E_g^2 + C_i)B_i^2 - 2E_gC_i]$; $Q_i = (1/2)(4C_i - B_i^2)^{1/2}$. Forouhi and Bloomer provide a table of FB coefficients, A_i, B_i, C_i, and E_g, for four terms in the summation in Equation (1.18) [1.39] for a number of semiconductors; an example that shows an excellent agreement between the FB dispersion relation and the experimental data is shown in Figure 1.3. Table 4 provides the FB coefficients for a few selected semiconductors. The reader is referred to Adachi's recent book and his papers for further discussions and other models on the refractive index of crystalline and amorphous semiconductors [1.10, 1.11, 1.41–1.44]; the optical properties of amorphous semiconductors are treated in a later chapter of this book.

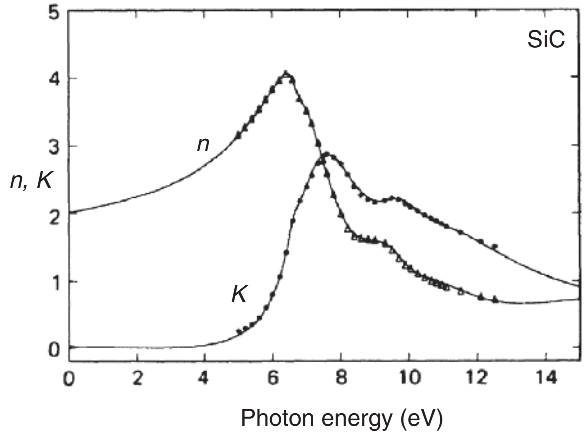

Figure 1.3 n and K versus photon energy for crystalline SiC. The solid line is obtained from the FB equation with four terms with appropriate parameters, and points represent the experimental data. See original reference [1.39] for details [Reprinted with permission Fig. 2c, A.R. Forouhi and I. Bloomer, *Phys. Rev. B*, **38**, 1865. Copyright (1988) by the American Physical Society]

Table 1.4 FB coefficients for selected semiconductors [1.39] for four terms $i = 1$ to 4. First entry in the box is for $i = 1$, and the fourth is for $i = 4$

	A_i	B_i (eV)	C_i (eV^2)	$n(\infty)$	E_g(eV)
Si	0.00405	6.885	11.864	1.950	1.06
	0.01427	7.401	13.754		
	0.06830	8.634	18.812		
	0.17488	10.652	29.841		
Ge	0.08556	4.589	5.382	2.046	0.60
	0.21882	6.505	11.486		
	0.02563	8.712	19.126		
	0.07754	10.982	31.620		
GaP	0.00652	7.469	13.958	2.070	2.17
	0.14427	7.684	15.041		
	0.13969	10.237	26.567		
	0.00548	13.775	47.612		
GaAs	0.00041	5.871	8.619	2.156	1.35
	0.20049	6.154	9.784		
	0.09688	9.679	23.803		
	0.01008	13.232	44.119		
GaSb	0.00268	4.127	4.267	1.914	0.65
	0.34046	4.664	5.930		
	0.08611	8.162	17.031		
	0.02692	11.146	31.691		
InP	0.20242	6.311	10.357	1.766	1.27
	0.02339	9.662	23.472		
	0.03073	10.726	29.360		
	0.04404	13.604	47.602		
InAs	0.18463	5.277	7.504	1.691	0.30
	0.00941	9.130	20.934		
	0.05242	9.865	25.172		
	0.03467	13.956	50.062		
InSb	0.00296	3.741	3.510	1.803	0.12
	0.22174	4.429	5.447		
	0.06076	7.881	15.887		
	0.04537	10.765	30.119		

B. Bandgap and temperature dependence

The refractive index of a semiconductor (typically for $\hbar\omega < E_g$) typically decreases with increasing energy bandgap E_g. There are various empirical and semi-empirical rules and expressions that relate n to E_g. Based on an atomic model, Moss has suggested that n and E_g are related by $n^4 E_g = K =$ constant (K is about ~100 eV). In the Hervé–Vandamme relationship [1.45],

$$n^2 = 1 + \left(\frac{A}{E_g + B}\right)^2 \tag{1.19}$$

where A and B are constants as $A \approx 13.6\,\text{eV}$ and $B \approx 3.4\,\text{eV}$. The temperature dependence of n arises from the variation of E_g with the temperature T and typically it increases with increasing temperature. The temperature coefficient of refractive index (TCRI) of semiconductors can be found from the Hervé–Vandamme relationship as:

$$\text{TCRI}=\frac{1}{n}\cdot\frac{\mathrm{d}n}{\mathrm{d}T}=\frac{(n^2-1)^{3/2}}{13.6n^2}\left[\frac{\mathrm{d}E_g}{\mathrm{d}T}+\frac{\mathrm{d}B}{\mathrm{d}T}\right] \tag{1.20}$$

where $\mathrm{d}B/\mathrm{d}T \approx 2.5 \times 10^{-5}\,\text{eV}\,\text{K}^{-1}$. TCRI is typically found to be in the range of 10^{-6} to $10^{-4}\,\text{K}^{-1}$.

1.3.4 Gladstone–Dale formula and oxide glasses

The Gladstone–Dale formula is an empirical equation that allows the average refractive index n of an oxide glass to be calculated from its density ρ and its constituents as:

$$\frac{n-1}{\rho}=p_1k_1+p_1k_1+\ldots=\sum_{i=1}^{N}p_ik_i=C_{\text{GD}} \tag{1.21}$$

where the summation is for various oxide components (each a simple oxide), p_i is the weight fraction of the i-th oxide in the compound, and k_i is the refraction coefficient that represents the polarizability of the i-th oxide. The right-hand side of Equation (1.21) is called the *Gladstone–Dale* coefficient C_{GD}. In more general terms, as a mixture rule for the overall refractive index, the Gladstone–Dale formula is frequently written as:

$$\frac{n-1}{\rho}=\frac{n_1-1}{\rho_1}w_1+\frac{n_2-1}{\rho_2}w_2+\cdots \tag{1.22}$$

where n and ρ are the effective refractive index and effective density, respectively, of the whole mixture, n_1, n_2, . . . are the refractive indices of the constituents, and ρ_1, ρ_2, . . . represent the densities of each constituent. Gladstone–Dale equations for the polymorphs of SiO_2 and TiO_2 give the average n, respectively, as [1.46, 1.47]:

$$n(\text{SiO}_2)=1+0.21\rho \quad\text{and}\quad n(\text{TiO}_2)=1+0.40\rho \tag{1.23}$$

1.3.5 Wemple–DiDomenico dispersion relation

Based on the single-oscillator model, the Wemple–DiDomenico is a semi-empirical dispersion relation for determining the refractive index at photon energies below the interband absorption edge in a variety of materials. It is given by:

$$n^2=1+\frac{E_oE_d}{E_o^2-(h\nu)^2} \tag{1.24}$$

where ν is the frequency, h is the Planck constant, E_o is the single-oscillator energy, E_d is the dispersion energy which is a measure of the average strength of interband optical transitions; $E_d = \beta N_c Z_a N_e$ (eV), where N_c is the effective coordination number of the cation nearest-neighbour to the anion (e.g., $N_c = 6$ in NaCl, $N_c = 4$ in Ge), Z_a is the formal chemical valency of the anion ($Z_a = 1$ in NaCl; 2 in Te; and 3 in GaP), N_e is the effective number of valence electrons per anion excluding the cores ($N_e = 8$ in NaCl, Ge; 10 in TlCl; 12 in Te; $9\frac{1}{3}$ in As_2Se_3), and β is a constant that depends on whether the interatomic bond is ionic (β_i) or covalent (β_c): $\beta_i = 0.26 \pm 0.04$ eV for (e.g., halides NaCl, ThBr, etc. and most oxides, Al_2O_3, etc.), $\beta_c = 0.37 \pm 0.05$ eV for (e.g., tetrahedrally bonded $A^N B^{8-N}$ zinc blende-and diamond-type structures, GaP, ZnS, etc., and wurtzite crystals have a β-value that is intermediate between β_i and β_c). Further, empirically, $E_o = CE_g(\mathrm{D})$, where $E_g(\mathrm{D})$ is the *lowest* direct bandgap and C is a constant; typically $C \approx 1.5$. E_o has been associated with the main peak in the $\varepsilon_r''(h\nu)$ versus $h\nu$ spectrum. The parameters required for calculating n from Equation (1.24) are listed in Table 5 [1.48]. While it is apparent that the Wemple–DiDomenico relation can only be approximate, it has nonetheless found wide acceptance among experimentalists due to its straightforward simplicity.

Table 1.5 Examples of parameters for Wemple–DiDomenico dispersion relationship [Equation (1.24)] in various materials [1.48]

Material	N_c	Z_a	N_e	E_o (eV)	E_d (eV)	β (eV)	β	Comment
NaCl	6	1	8	10.3	13.6	0.28	β_i	Halides, LiF, NaF, etc
CsCl	8	1	8	10.6	17.1	0.27	β_i	CsBr, CsI, etc
TlCl	8	1	10	5.8	20.6	0.26	β_i	TlBr
CaF_2	8	1	8	15.7	15.9	0.25	β_i	BaF_2, etc
CaO	6	2	8	9.9	22.6	0.24	β_i	Oxides, MgO, TeO_2, etc
Al_2O_3	6	2	8	13.4	27.5	0.29	β_i	
$LiNbO_3$	6	2	8	6.65	25.9	0.27	β_i	
TiO_2	6	2	8	5.24	25.7	0.27	β_i	
ZnO	4	2	8	6.4	17.1	0.27	β_i	
ZnSe	4	2	8	5.54	27.0	0.42	β_c	II–VI, Zinc blende, ZnS, ZnTe,CdTe
GaAs	4	3	8	3.55	33.5	0.35	β_c	III–V, Zinc blende, GaP, etc
Si (Crystal)	4	4	8	4.0	44.4	0.35	β_c	Diamond, covalent bonding; C (diamond), Ge, β-SiC etc
SiO_2 (Crystal)	4	2	8	13.33	18.10	0.28	β_i	Average crystalline form
SiO_2 (Amorphous)	4	2	8	13.38	14.71	0.23	β_i	Fused silica
CdSe	4	2	8	4.0	20.6	0.32	β_i–β_c	Wurtzite

1.3.6 Group index

Group index is a factor by which the group velocity of a group of waves in a dielectric medium is reduced with respect to propagation in free space. It is denoted by N_g and defined by $N_g = v_g/c$, where v_g is the group velocity, defined by $v_g = d\omega/dk$ where k is the wave vector or the propagation constant. The group index can be determined from the ordinary refractive index n through:

$$N_g = n - \lambda \frac{dn}{d\lambda} \tag{1.25}$$

where λ is the wavelength of light. Figure 1.4 illustrates the relation between N_g and n in SiO_2. The group index N_g is the quantity that is normally used in calculating dispersion in optical fibers since it is N_g that determines the group velocity of a propagating light pulse in a glass or transparent medium. It should be remarked that although n versus λ can decrease monotonically with λ over a range of wavelengths, N_g can exhibit a minimum in the same range where the dispersion, $dN_g/d\lambda$, becomes zero. The point $dN_g/d\lambda = 0$ is called the zero-material *dispersion wavelength*, which is around 1300 nm for silica as is apparent in Figure 1.4.

1.4 THE SWANEPEL TECHNIQUE: MEASUREMENT OF n AND α

1.4.1 Uniform-thickness films

In many instances, the optical constants are conveniently measured by examining the transmission through a thin film of the material deposited on a transparent glass or other (e.g.,

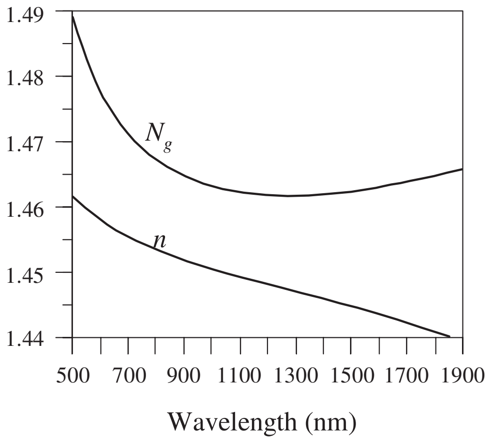

Figure 1.4 Refractive index n and the group index N_g of pure SiO_2 (silica) glass as a function of wavelength [Reproduced with permission from S.O. Kasap, *Principles of Electronic Materials and Devices*, 3rd Edition, McGraw-Hill, Boston, 2005]

sapphire) substrate. The classic reference on the optical properties of thin films has been the book by Heavens [1.49]; the book is still useful in clearly describing what experiments can be carried out, and has a number of useful derivations such as the reflectance and transmittance through thin films in the presence of multiple reflections. Since then numerous research articles and reviews have been published. Poelmen and Smet [1.50] have critically reviewed how a single transmission spectrum measurement can be used to extract the optical constants of a thin film. In general, the amount of light that gets transmitted through a thin film material depends on the amount of reflection and absorption that takes place along the light path. If the material is a thin film with a moderate absorption coefficient α then there will be multiple interferences at the transmitted side of the sample, as illustrated in Figure 1.5.

In this case, some interference fringes will be evident in the transmission spectrum obtained from a spectrophotometer, as shown in Figure 1.6. One very useful method that makes use of these interference fringes to determine the optical properties of the material is called the *Swanepoel method* [1.51].

Swanepoel has shown that the optical properties of a uniform thin film of thickness d, refractive index n, and absorption coefficient α, deposited on a substrate with a refractive index s, as shown in Figure 1.5, can be obtained from the transmittance T given by:

$$T = \frac{Ax}{B - Cx\cos\varphi + Dx^2} \tag{1.26}$$

where $A = 16n^2s$, $B = (n + 1)^3(n + s^2)$, $C = 2(n^2 - 1)(n^2 - s^2)$, $D = (n^2 - 1)^3(n - s^2)$, $\varphi = 4\pi nd/\lambda$, $x = \exp(-\alpha d)$ is the absorbance, and n, s, and α are all function of wavelength, λ. What is very striking and useful is that all the important optical properties can be determined from the application of this equation; these will be introduced in the subsequent paragraphs. Before optical properties of any thin films can be extracted, the refractive index of

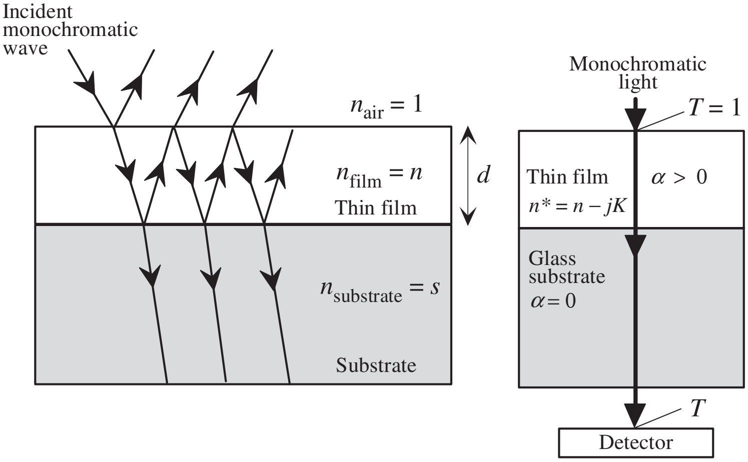

Figure 1.5 Schematic sketch of the typical behavior of light passing through a thin film on a substrate. On the left, oblique incidence is shown to demonstrate the multiple reflections. In most measurements, the incident beam is nearly normal to the film as shown on the right

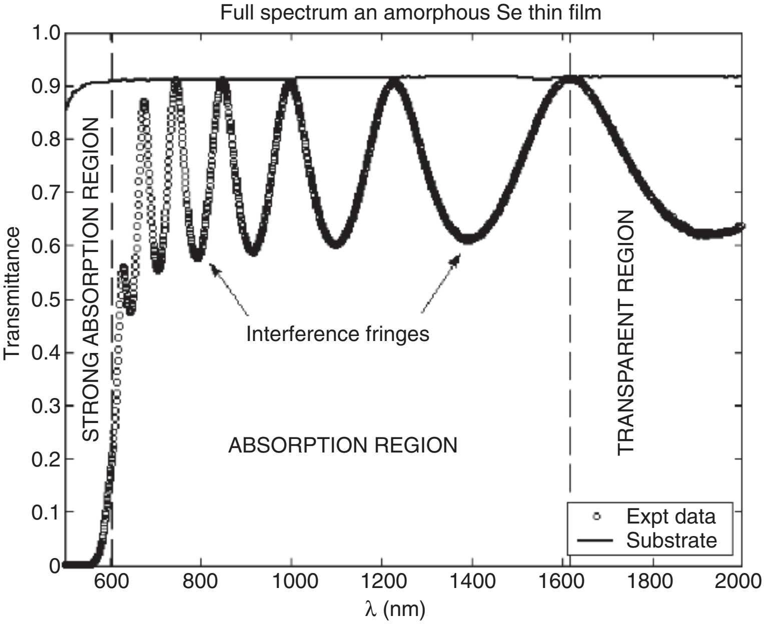

Figure 1.6 An example of a typical transmission spectrum of a 0.969 μm thick amorphous Se thin film that has been vacuum coated onto a glass substrate held at a substrate temperature of 50 °C during the deposition

their substrate must first be calculated. For a glass substrate with very negligible absorption, $K \leq 0.1$ and $\alpha \leq 10^{-2}\,\mathrm{cm}^{-1}$, in the range of the operating wavelengths, the refractive index s is:

$$s = \frac{1}{T_s} + \sqrt{\left(\frac{1}{T_s^2} - 1\right)} \tag{1.27}$$

where T_s is the transmittance value measured from a spectrophotometer. This expression can be derived from the transmittance equation for a bulk sample with little attenuation. With this refractive index s, the next step is to construct two envelopes around the maxima and minima of the interference fringes in the transmission spectrum as indicated in Figure 1.7.

There will altogether be two envelopes that have to be constructed before any of the expressions derived from Equation (1.26) can be used to extract the optical properties. This can be done by locating all the extreme points of the interference fringes in the transmission spectrum and then making sure that the respective envelopes, $T_M(\lambda)$ for the maxima and $T_m(\lambda)$ for the minima, pass through these extremes, the maxima and minima, of $T(\lambda)$ tangentially. From Equation (1.26), it is not difficult to see that at $\varphi = \pm 1$, the expressions that describe the two envelopes are:

$$T_M = \frac{Ax}{B - Cx + Dx^2} \tag{1.28a}$$

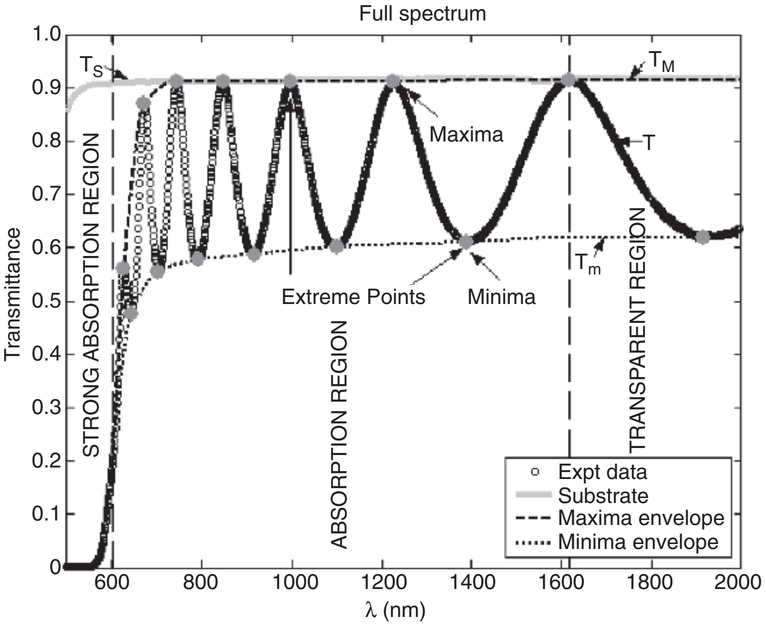

Figure 1.7 The construction of envelopes in the transmission spectrum of the thin amorphous Se film in Figure 1.5

$$T_m = \frac{Ax}{B + Cx + Dx^2} \tag{1.28b}$$

Figure 1.7 shows two envelopes constructed for a transmission spectrum of an amorphous Se thin film. It can also be seen that the transmission spectrum has been divided into three special regions according to their transmittance values: (i) the *transparent region*, where $T(\lambda) \geq 99.99\%$ of the substrate's transmittance value of $T_s(\lambda)$, (ii) the *strong-absorption region*, where $T(\lambda)$ is typical smaller than 20% of $T_s(\lambda)$, and (iii) the *absorption region*, in between the two latter regions as shown in Figure 1.7:

The refractive index of the thin film can be calculated from the two envelopes, $T_M(\lambda)$ and $T_m(\lambda)$, and the refractive index of the substrate s through

$$n = \left[N + (N^2 - s^2)^{1/2}\right]^{1/2}; \quad N = 2s\left[\frac{T_M - T_m}{T_M T_m}\right] + \frac{s^2 + 1}{2} \tag{1.29}$$

where N is defined by the second equation above. Since the equation is not valid in the strong-absorption region, where there are no maxima and minima, the calculated refractive index has to be fitted to a well established dispersion model for extrapolation to shorter wavelengths before it can be used to obtain other optical constants. Usually either the Sellmeier or the Cauchy dispersion equation is used to fit n versus λ experimental data in this range. Figure 1.8 shows the refractive indices extracted from the envelopes and a fitted Sellmeier dispersion model with two terms.

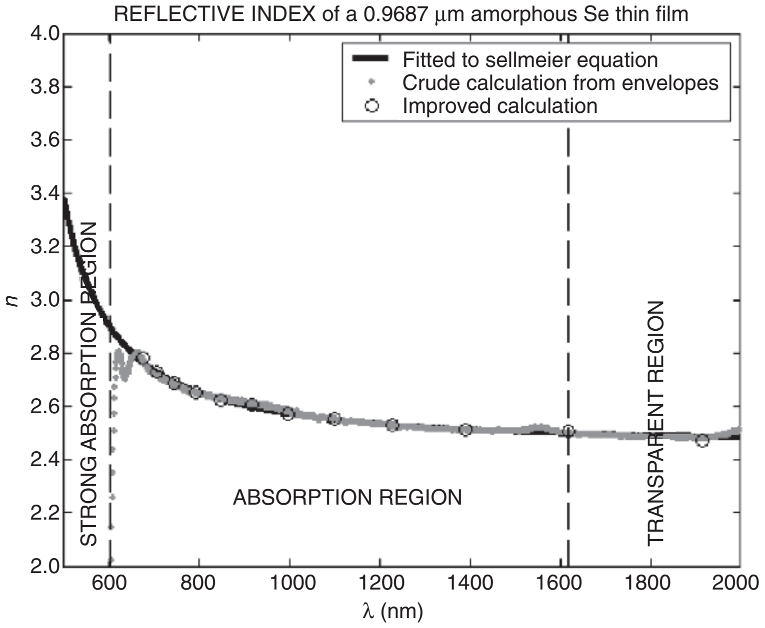

Figure 1.8 Determination of the refractive index from the transmission spectrum maxima and minima shown in Figure 1.6. The fitted Sellmeier n vs λ curve follows $n^2 = 3.096 + 2.943\lambda^2/[\lambda^2 - (4.02310^{-7})^2]$

With the refractive index of the thin film corresponding to two adjacent maxima (or minima) at points 1 and 2 given as n_1 at λ_1 and n_2 at λ_1, the thickness can be easily calculated from the basic interference equation of waves as follows:

$$d_{\text{crude}} = \frac{\lambda_1 \lambda_2}{2(\lambda_1 n_2 - \lambda_2 n_1)} \tag{1.30}$$

where d_{crude} refers to the thickness obtained from the maxima (minima) at points 1, 2. As other adjacent pairs of maxima or minima points are used, more thickness values can be deduced, and hence an average value calculated. It is assumed the film has an ideal uniform thickness.

The absorption coefficient α can be obtained once the absorbance x is extracted from the transmission spectrum. This can be done as follows:

$$\alpha = -\frac{\ln(x)}{d_{\text{ave}}} \tag{1.31}$$

where $x = \dfrac{E_M - \sqrt{E_M^2 - (n^2-1)^3(n^2-s^4)}}{(n-1)^3(n-s)^2}$; $E_M = \dfrac{8n^2 s}{T_M} + (n^2-1)(n^2-s^2)$ and d_{ave} is the average thickness of d_{crude}.

The accuracy of the thickness, the refractive index, and the absorption coefficient can all be further improved in the following manner. The first step is to determine a new set of interference orders number, m', for the interference fringes from the basic interference equation of waves, that is:

$$m' = \frac{2n_e d_{\text{ave}}}{\lambda_e} \tag{1.32a}$$

where n_e and λ_e are values taken at any extreme points, and m' is an integer if the extremes taken are maxima, or a half-integer if the extremes taken are minima.

The second step is to get a new corresponding set of thickness, d', from this new set of order numbers m', by rearranging Equation (1.32a) as:

$$d' = \frac{m'\lambda_e}{2n_e} \tag{1.32b}$$

From this new set of thicknesses, d', a new average thickness, d_{new}, must be calculated before it can applied to improve the refractive index. With this new average thickness, a more accurate refractive index can be obtained from the same equation:

$$n_e' = \frac{m'\lambda_e}{2d_{\text{new}}} \tag{1.32c}$$

This new refractive index can then be fitted to the previous dispersion model again so that an improved absorption coefficient α can be calculated from Equation (1.31). All these parameters can then be used in Equation (1.26) to regenerate a transmission spectrum $T_{\text{cal}}(\lambda)$ so that the root mean square error (RMSE) can be determined from the experimental spectrum T_{exp}. The RMSE is calculated as follows:

$$\text{RMSE}=\sqrt{\frac{\sum_{i=1}^{q}(T_{\text{exp}} - T_{\text{cal}})^2}{q}} \tag{1.33}$$

where T_{exp} is the transmittance of the experimental or measured spectrum, T_{cal} is the transmittance of the regenerated spectrum using the Swanepoel calculation method, and q is the range of the measurement. Figure 1.9 shows the regenerated transmission spectrum of the amorphous Se thin film that appeared in Figure 1.6 using the optical constants calculated from the envelopes.

1.4.2 Thin films with nonuniform thickness

For a film with a wedge-like cross-section as shown in Figure 1.10, Equation (1.26) must be integrated over the thickness of the film in order for it to more accurately describe the transmission spectrum [1.52]. The transmittance then becomes

$$T_{\Delta d} = \frac{1}{\varphi_2 - \varphi_1} \int_{\varphi_1}^{\varphi_2} \frac{Ax}{B - Cx\cos\varphi + Dx^2} dx \tag{1.34}$$

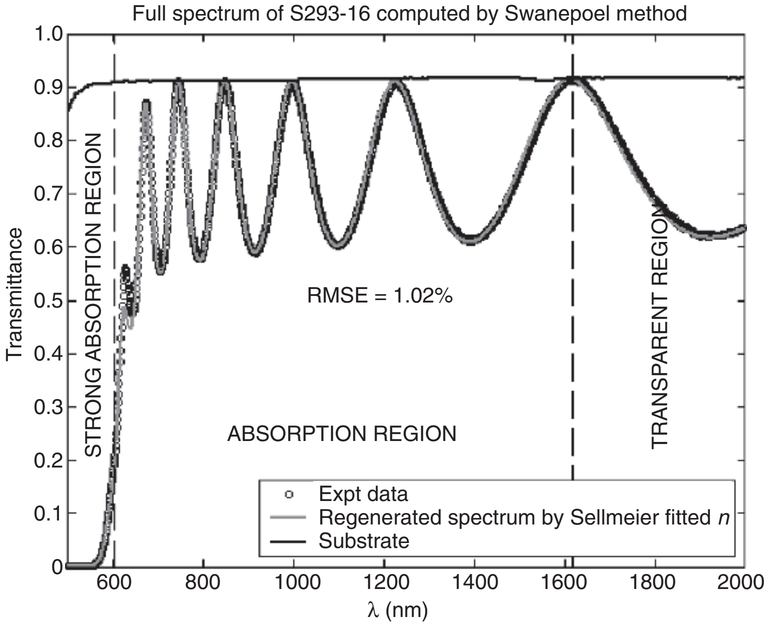

Figure 1.9 Regenerated transmission spectrum of the sample in Figure 1.6

with $\varphi_1 = \dfrac{4\pi n(\bar{d} - \Delta d)}{\lambda}$, *and* $\varphi_2 = \dfrac{4\pi n(\bar{d} + \Delta d)}{\lambda}$, where $A = 16n^2 s$, $B = (n+1)^3(n+s^2)$, $C = 2(n^2-1)(n^2-s^2)$, $D = (n-1)^3(n-s^2)$, $x = \exp(-\alpha d)$ is the absorbance, n and s are the refractive index of the film and substrate respectively, α the absorption coefficient, $\bar{d}$ is the average thickness of the film, and Δd is the *thickness variation* throughout the illumination area, which has been called the *roughness* of the film. (This nomenclature is actually confusing since the film may not be truly 'rough' but may just have a continuously increasing thickness as in a wedge from one end to the other.)

The first parameter to be extracted before the rest of the optical properties is Δd. Since the integration in Equation (1.34) cannot be carried out from one branch of the tangent to another, it cannot be used directly in this form. The equation was thus modified by considering the maxima and minima, which are both continuous function of λ, in a case-by-case basis. In this way, we have

Maxima: $$T_{Md} = \frac{\lambda}{2\pi n \Delta d} \frac{a}{\sqrt{1-b^2}} \tan^{-1}\left[\frac{1+b}{\sqrt{1-b^2}} \tan\left(\frac{2\pi n \Delta d}{\lambda}\right)\right] \quad (1.35a)$$

Minima: $$T_{md} = \frac{\lambda}{2\pi n \Delta d} \frac{a}{\sqrt{1-b^2}} \tan^{-1}\left[\frac{1-b}{\sqrt{1-b^2}} \tan\left(\frac{2\pi n \Delta d}{\lambda}\right)\right] \quad (1.35b)$$

where $a = \dfrac{A}{B+D}$, and $b = \dfrac{C}{B+D}$. As long as $0 < \Delta d < \lambda/4n$, the refractive index, n, and Δd can both be obtained simultaneously by solving Equation (1.35a) and (1.35b) numerically.

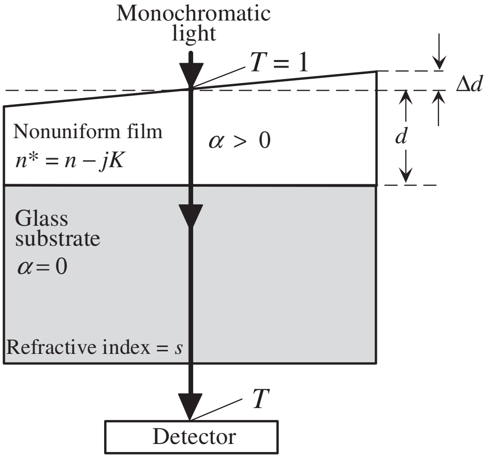

Figure 1.10 System of an absorbing thin film with a variation in thickness on a thick finite transparent substrate

Since Equations (1.35a) and (1.35b) are only valid in the region of zero absorption, the refractive index outside the transparent region must be obtained in another way. Theoretically, a direct integration of Equation (1.34) over both Δd and x can be performed, though this would be analytically too difficult; nevertheless, an approximation to the integration is also possible as follows:

Maxima: $$T_{Mx} = \frac{\lambda}{2\pi n\Delta d}\frac{a_x}{\sqrt{1-b_x^2}}\tan^{-1}\left[\frac{1+b_x}{\sqrt{1-b_x^2}}\tan\left(\frac{2\pi n\Delta d}{\lambda}\right)\right] \tag{1.36a}$$

Minima: $$T_{mx} = \frac{\lambda}{2\pi n\Delta d}\frac{a_x}{\sqrt{1-b_x^2}}\tan^{-1}\left[\frac{1-b_x}{\sqrt{1-b_x^2}}\tan\left(\frac{2\pi n\Delta d}{\lambda}\right)\right] \tag{1.36b}$$

where $a = \frac{Ax}{B+Dx^2}$, and $b = \frac{Cx}{B+Dx^2}$. As long as $0 < x \le 1$, numerically, there will only be one unique solution. Therefore the two desired optical properties, refractive index, n, and the absorbance, x, can both be obtained when Equations (1.36a) and (1.36b) are solved simultaneously using the calculated average Δd.

As before, the calculated refractive index can be fitted to a well established dispersion model, such as the Cauchy or Sellmeier equation, for extrapolation to shorter wavelengths and the thickness is calculated from any two adjacent maxima (or minima) using Equation (1.30). Given that the absorbance, from Equations (1.36a) and (1.36b) is not valid in the strong-absorption region, the absorption coefficient outside this region is calculated differently from those in the strong region as:

$$\alpha_{\text{out}} = -\frac{\ln(x_{\text{out}})}{d_{\text{ave}}} \tag{1.37}$$

where x_{out} is the absorbance obtained from Equations (1.36a) and (1.36b) and d_{ave} is the average thickness.

According to Swanepoel, in the region of strong absorption, the interference fringes are smaller and the spectrum approaches the interference-free transmission sooner. Since the transmission spectra in this region are the same for any film with the same average thickness, regardless of its uniformity, the absorption coefficient in the strong region will thus be

$$\alpha_{\text{strong}} = -\frac{\ln(x_{\text{strong}})}{d_{\text{ave}}} \tag{1.38}$$

where $x_{\text{strong}} = \dfrac{A - \sqrt{(A^2 - 4T_i^2 BD)}}{2T_i D}$, $T_i = \dfrac{2T_M T_m}{T_M + T_m}$, and T_M and T_m are the envelopes constructed from the measured spectrum.

The accuracy of the thickness and refractive index can be further improved in exactly the same way as for a uniform thickness film and used for the computation of the new refractive index and absorption coefficient using Equations (1.36a) and (1.36b). Figure 1.11 shows the regenerated transmission spectrum of a simulated sample with nonuniform thickness using the optical constants calculated from the envelopes. Marquez et al. [1.53] have discussed the application of the Swanepoel technique to wedge-shaped As_2S_3 thin films and made use of the fact that a nonuniform wedge-shaped thin film has a compressed transmission spectrum.

Various computer algorithms that can be used to obtain n and K based on the Swanepoel technique are available in the literature [1.54]. Further discussions and enhancements are

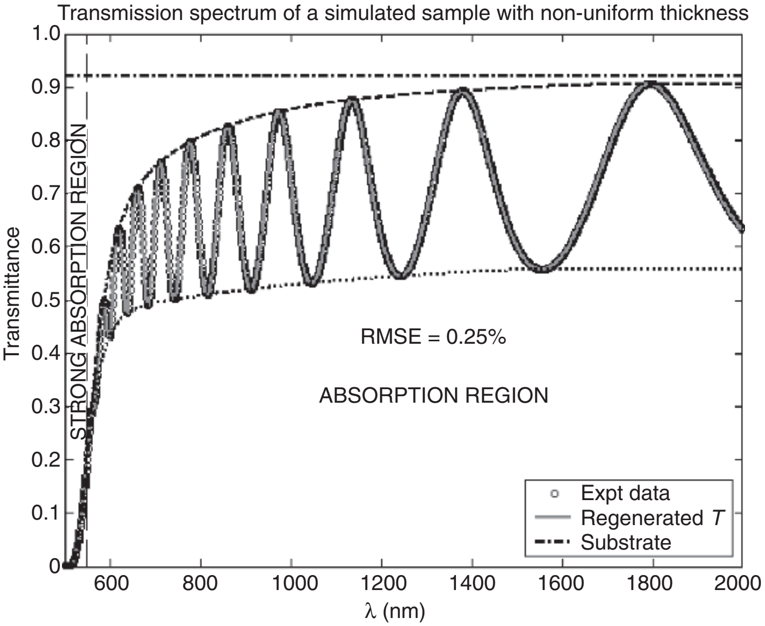

Figure 1.11 A regenerated transmission spectrum of a sample with an average thickness of 1 μm, average Δd of 30 nm, and a refractive index fitted to a Cauchy equation in Figure 1.12

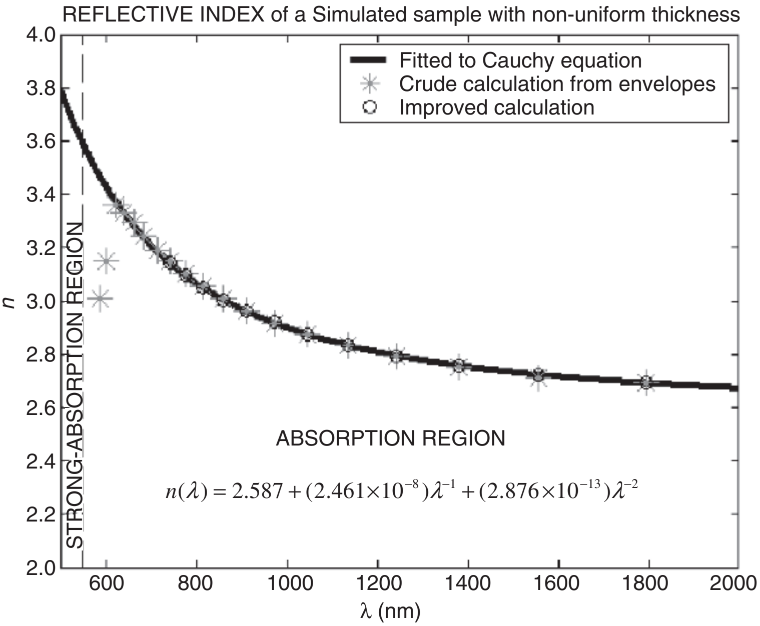

Figure 1.12 The refractive index of a sample with $\bar{d} = 1\ \mu\text{m}$ and $\Delta d = 30\,\text{nm}$, and n fitted to a Cauchy equation

also available in the literature [1.50, 1.55, 1.56]. There are numerous useful applications of the Swanepoel technique for extracting the optical constants of thin films; some selected recent examples are given in [1.57–1.67].

1.5 CONCLUSIONS

This chapter has provided a semiquantitative explanation and discussion of the complex refractive index $n^* = n - jK$, the relationship between the real n and imaginary part K through the Kramers–Kronig relationships, various common dispersion (n versus λ) relationships such as the Cauchy, Sellmeier, Wemple–DiDomenico dispersion relations, and the determination of the optical constants of a material in thin film form using the popular Swanepoel technique. Examples are given to highlight the concepts and provide applications. Optical constants of various selected materials have also been provided in tables to illustrate typical values and enable comparisons to be made.

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