Calculation of refractive index of some materials

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Abstract - The refractive index of semiconductors thin films is an important parameter for the design of waveguides, modulators, detectors and lasers. We present in this paper a temperature dependent Sellmeier equation for the refractive index of Zinc Selenide and Silicon. The refractive index is given at wavelengths of 0.5 µm and 0.7 µm for ZnSe and Si respectively. The temperature-dependent refractive index dispersion profiles for both of them are given for range temperatures of 50-300 K. We used Sellmeier coefficients previously published for calculations. Our results are in good agreement with experimental ones.

1. INTRODUCTION

The refractive index of a material is the most important of any optical system that uses refraction. It is used to calculate the focusing power of lenses, and the dispersive power of prisms. Since refractive index is a fundamental physical property of a substance. It is often used to identify a particular substance, confirm its purity, or measure its concentration. It is used to measure solids (glasses and gemstones), liquids, and gases [1].

In this paper we calculate refractive index of two semiconductors: ZnSe and Si, using Sellmeier equation that describes their chromatic dispersion properties.

The Sellmeier equation is an empirical relationship between refractive index $n$ and wavelength $\lambda$ for particular transparent medium, using the result for $\chi$ for Lorentz oscillators as basis functions [2]. It is convenient to use and quite simple, so one can analyze any structures with accuracy. However, it is only valid for room temperature. Hence, Sellmeier equations are of the form:

$$n^2(\omega) = 1 + \sum_j \frac{\omega_j^2}{\omega_0^2 - \omega_j^2}$$

These equations are very useful ways of providing data on the refractive index of materials vs. wavelength, without the need for extensive tables. They are usually valid only in high transparency spectral regions, far from resonances, where $\chi$ is real. Often, but not always, Sellmeier equation for a material may contain a pole (i.e. a resonance) at low frequency ($\omega_0 \ll \omega$) and one at very high frequency ($\omega_0 \ll \omega$). Hence one could write:

$$n^2(\omega) = 1 + \frac{\omega_\infty^2}{\omega_0^2} + \sum_j \frac{\omega_j^2}{\omega_0^2 - \omega_j^2} - \frac{\omega_0^2}{\omega^2}$$

where, $1 + \frac{\omega_\infty^2}{\omega_0^2}$ is more commonly written as $\varepsilon_\infty$.

In practice, these equations are usually expressed in terms of wavelength:

$$n^2(\lambda) = 1 + A + \sum_j \frac{\lambda_j^2}{\lambda_0^2 - \lambda_j^2} - d\lambda^2 = a + \sum_j \frac{b_j\lambda^2}{\lambda^2 - c_j} - d\lambda^2$$

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so that coefficients $a$, $b_j$, $c_j$, and $d$ may completely describe the refractive index vs. wavelength for a material, and $A = \frac{a_0^2}{\omega_0^2}$. There are usually only one or two values of $j$ (i.e. only one or two resonances) in the Sellmeier equation for a given material. This may depend on the material and on the level of accuracy required.

2. RESULTS AND DISCUSSIONS

2.1 ZnSe

Zinc selenide is a clear yellow polycrystalline material with a grain size of approximately 70 µm, transmitting in the range 0.5-22 µm. It is essentially free of extrinsic impurity absorptions, providing extremely low bulk losses from scatter. The main identifiable extrinsic bulk absorption is zinc hydride, whose free diatomic molecule has a vibrational mode at 1608 cm\(^{-1}\). Having a very low absorption of energy makes it useful for optical components in high power laser window and multispectral applications, providing good imaging characteristics. ZnSe is also useful in high resolution thermal imaging systems, where it is used to correct for colour distortion which is often inherent in other lenses used in the system [3]. An observed electronic absorption edge at approximately 0.476 µm (≈ 2.6 eV) at 300 K and far infrared multi-phonon absorption edge commencing at approximately 22.2 µm.

The multi-phonon lattice absorption of ZnSe has been extensively investigated since the first transmission and reflection measurements were made by Aven et al. on cubic ZnSe in 1961. Since neutron-cattering and Raman-scattering have become available in the early 1970’s, as has the increased availability of CVD ZnSe, investigations of ZnSe has demonstrated that in the three and four-phonon regions, ZnSe exhibits a characteristic structure consistent with predicted calculations by Bendow et al [4].

At wavelengths between the visible and infrared regions, ZnSe behaves as a dielectric material, with a refractive index decreasing with increasing wavelength. The mean value of $n$ being approximately 2.4 at 300 K. Over this same region, the extinction coefficient $k$ is very small ($< 10^{-5}$), providing uniformly high transmission. As a result of these characteristics, ZnSe has been used extensively for optical components and windows. Marple et al. [5] derived the following Sellmeier type dispersion equation at 300 K with a claimed experimental error of ± 0.002:

$$n^2 = \frac{4.0 + \frac{1.90 \lambda^2}{\lambda^2 - 0.0113}}{\lambda^2}$$

<table>
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<th>Wave length, µm</th>
<th>2.75</th>
<th>5.00</th>
<th>7.50</th>
<th>9.50</th>
<th>11.0</th>
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<td>2.44</td>
<td>2.43</td>
<td>2.42</td>
<td>2.41</td>
<td>2.40</td>
<td>2.39</td>
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<table>
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<tr>
<th>Wave length, µm</th>
<th>15.0</th>
<th>16.0</th>
<th>16.9</th>
<th>17.8</th>
<th>18.6</th>
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<tbody>
<tr>
<td>Refractive Index</td>
<td>2.37</td>
<td>2.36</td>
<td>2.35</td>
<td>2.34</td>
<td>2.33</td>
<td>2.32</td>
<td>2.31</td>
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</table>

2.2 Si

Silicon is used as an optical window primarily in the 3 to 5 microns band and as a substrate for production of optical filters. It is frequently used for laser mirrors because of its high thermal conductivity and low density. Silicon is also useful as a transmitter in the 20 microns range. Large blocks with polished faces are also employed as targets in neutron physics experiments. Silicon is grown by Czochralski pulling techniques (CZ) and contains some oxygen which causes an
absorption band at 9 microns. To avoid this, material can be prepared by a Float-Zone (FZ) process. Optical silicon is generally lightly doped (5 to 40 ohm cm) for best transmission above 10 microns. Silicon has a further pass band 30 to 100 microns which is effective only in very high resistivity uncompensated material [6].

![Graph showing percentage transmittance vs. wavelength for ZnSe](image1)

**Fig. 1:** Percentage transmittance vs. wavelength for ZnSe

![Graph showing refractive index vs. wavelength at 0.5 µm](image2)

**Fig. 2:** Refractive index vs. wavelength at 0.5 µm. The refractive index of ZnSe at 0.5 µm is 2.741

![Graph showing temperature-dependent refractive index dispersion profile for CVD (ZnSe)](image3)

**Fig. 3:** Temperature-dependent refractive index dispersion profile for CVD (ZnSe)

The refractive index of the transparent region of silicon has been reported by a number of investigators using a variety of techniques. Each of these reports has found variations in accuracy such that no coherent set of temperature dependent dispersion profiles have emerged even though high purity optical quality single crystal material was used. Consequently, the refractive index
data derived for a temperature-dependent predictive dispersion model is the result of selective data across different wavelength regions.

The following dispersion equation producing the best fit to this disparate data set for ambient room temperature (293 K) was derived by Edwards et al. [7] with the following modified Sellmeier expression.

\[ n^2 = \varepsilon + \frac{A}{\lambda^2} + \frac{B \lambda_1^2}{\lambda^2 - \lambda_1^2} \]

where \( \lambda_1 = 1.1071 \mu \text{m} \), \( \varepsilon = 1.16858 \times 10^4 \), \( A = 9.39816 \times 10^{-1} \) and \( B = 8.10461 \times 10^{-3} \).

Fig. 4: Percentage transmittance vs. wavelength for Si

\[ n^2 = \varepsilon + \frac{A}{\lambda^2} + \frac{B \lambda_1^2}{\lambda^2 - \lambda_1^2} \]

The refractive index of Si at 0.7 \( \mu \text{m} \) is 3.782

Fig. 5: Refractive index vs. wavelength at 0.7 \( \mu \text{m} \).

Fig. 6: Temperature-dependent refractive index dispersion profile for (Si)
### Table 2: Experimental results for Si

<table>
<thead>
<tr>
<th>Wave length, µm</th>
<th>1.40</th>
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<th>1.66</th>
<th>1.82</th>
<th>2.05</th>
<th>2.50</th>
<th>3.50-5.00</th>
<th>6.00-25.0</th>
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<tbody>
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<td>Refractive Index</td>
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<td>3.45</td>
<td>3.44</td>
<td>3.43</td>
<td>3.42</td>
</tr>
</tbody>
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### 3. CONCLUSION

Sellmeier data are very useful to evaluate the dispersion of a material. This involves frequency derivatives, which can be performed analytically or numerically, and are unproblematic with Sellmeier data even for high orders of dispersion.

The literature contains a great variety of modified formulae which are also often called Sellmeier formulae. Extensions to the simple form given above can enlarge the wavelength range of validity, and allow to describe the temperature dependence of refractive indices.

In this paper we obtained interesting results about refractive index and temperature-dependent refractive index dispersion profile for both of ZnSe and Si.

### REFERENCES