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DETERMINATION OF SPECTRAL OPTICAL CONSTANTS OF GLAZINGS BY NUMERICAL INTEGRATION FROM FTIR SPECTROMETER MEASUREMENTS

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Abstract.*The correct characterization of different materials assists in improving the results obtained via physical and numerical models. This study consists of the development of a numerical algorithm based on experimental data to obtain the spectral values of the index of refraction (n) and the coefficient of extinction* (k) *of several types of glasses available on the Brazilian market. An FTIR Spectrometer was used in the experimental stage. The real and imaginary parts of the complex index of refraction (*$\hat{n} = n + ik$*), were evaluated using the Kramers-Krönig relations and the respective numerical integration. The spectral values of the optical constants obtained as a result will be included in future studies to determine the radiative behavior of thin-film coatings on glass substrates.*

Keywords: *radiative properties , glazing systems, index of refraction , extinction coefficient , spectromerty*

1. INTRODUCTION

In order to improve the energy efficiency of a building, the trend to reduce energy losses through enclosures such as walls and windows is becoming an increasingly important matter. Adequate window design, selection, and orientation can reduce a building's heating power in cold climates and the cooling requirements in hot climates. Windows are thermally critical elements of the building envelope because they are difficult to insulate and produce much higher conductive gains and losses than corresponding wall areas. A very important characteristic of windows is the transmission of light (short wavelength thermal radiation) directly into the thermal zone because it provides natural lighting inside the building. This transmitted radiation is usually a desirable heat gain in the winter and an undesirable gain in the summer. Thus, windows play a key role in the energy efficiency of both residential and commercial buildings. At least one-fourth of domestic heating requirements in OECD (Organization for Economic Co-operation and Development) countries are considered a direct result of energy losses through windows (Muneer and Kubie, 1999). In recent years, major efforts have been made to improve the thermal behavior of windows using various technologies, such as low-emissivity coatings, inert gas-filling, insulating edge spacers, low-conductivity frames, among others. This approach has led to windows with a thermal transmittance nearly as good as a wall (Urbikain *et al.*, 2007). Adequate window design, selection, and orientation can strongly reduce heating and cooling loads predicted by building simulation tools. In order to improve the accuracy of those tools, this study determines the spectral optical properties index of refraction (n) and the coefficient of extinction (k) using the spectral reflectance measurement as input according to FTIR Spectrometry. A numerical integration must be developed to obtain the phase angle (ϕ). The characterization of glasses and transparent elements, regarding radiative properties, are always necessary for Building Simulation and Energy Efficiency evaluation because when the physical properties are well defined, there is an improvement in the quality of the results. This study aims to determine the spectral optical properties, namely the index of refraction (n) and the coefficient of extinction (k) of some typical glass samples available in the Brazilian market and commonly regarded by energy simulation as generic and global values.

2. THEORETICAL BACKGROUND

This section includes a theoretical background for radiative properties of transparent media, as well as a mathematical approach addressing the dielectric properties n and k. Additionally, we reveal how the Kramers-Krönig formulation is used to evaluate the complex index of refraction and its constants (n and k) (Hecht, 2016).

2.1 Radiative properties

The radiative properties that concern energy evaluation for glasses are normally transmittance, reflectance, and absorptance, which correspond to the fraction of the impinging radiation that is transmitted, reflected, or absorbed, respectively (Howell *et al.*, 2010). These properties are wavelength dependent and can in many thorough cases be measured or theoretically analyzed. Factors such as sample geometry, homogeneity, or scattering, must be taken into account for both for theoretical calculations and measurements. The authors have considered such factors, and thus have employed an FTIR Spectrometer to obtain the spectral data in order to measure reflectance and subsequently, have determined the phase angle via numerical integration.

2.2 Solar optical properties

Silica glasses are partially transparent throughout the near-ultraviolet, visible, and near-infrared regions that compose the solar spectrum (0.3 - 3 μm) (Kitamura *et al.*, 2007). The transmittance and reflectance of these glasses vary much more in the solar spectrum than in the far-infrared due to the presence of ferrous oxide (FeO) in the raw materials added to control and melting. Other absorbers are added to produce other typical glasses known on the market as bronze, grey, and blue-green. Variations in chemical composition and deviations from nominal thickness result in small variations in spectral averaged transmittance. In some cases, the mean value of transmittance for a particular color and thickness varies by over 2% among manufacturers. Standard deviations are generally lower than 3% for each type of glass (Rubin, 1985). For a defined wavelength, the differences in transmittance can be much larger than the differences in total properties, especially near absorption peaks.

2.3 Glazing Optical Constants

The power reflection coefficient (ρ) was measured at near-normal incidence from 0.5 to μm with a Fourier-transform spectrometer. The phase angle (ϕ) of the amplitude reflection coefficient at frequency (ω), is related to ρ through the Kramers- Krönig formula (Hu, 1989):

$$\phi_\omega = \frac{\omega}{\pi}\int_0^\infty \frac{ln\rho\,(\omega')}{(\omega'^2-\omega^2)}d\omega'. \tag{1}$$

Then the real and imaginary parts of the complex index of refraction (n and k) are related to ρ and ϕ (Rubin, 1985):

$$n = \frac{1-\rho}{1-2\sqrt{\rho}\,cos\phi+\rho}, \tag{2}$$

$$k = \frac{2\sqrt{\rho}\,sin\phi}{1-2\sqrt{\rho}\,cos\phi+\rho}. \tag{3}$$

In theory, we would need ρ from ϕ = 0 to ∞, not solely from the region over which we would calculate the optical constants. We can justify some extrapolation because ρ does not vary dramatically, thus its contribution to the wavelength in question is minimal. This can be shown more clearly by integrating Eq. (1) by parts:

$$\phi_\omega = \frac{1}{2\pi}\int_0^\infty \frac{d\,ln\rho}{d\,\omega'}\,ln\left|\frac{\omega'+\omega}{\omega'-\omega}\right|d\omega'. \tag{4}$$

Equation (4) also shows that regions of constant ρ do not contribute to this integral. ρ is a small value that varies slowly between 0.3 and 3.0 μm. The optical constants in this transparent region are included in the next section. The values of k, defined by Bagdad and Stolen (1968) and highlighted by Rubin (1985), show that absorption is barely strong enough at 200 μm to affect ρ and that this effect decreases rapidly with increasing wavelength. Therefore, we may infer that ρ approaches a limiting value of 0.2 at 50 μm, in accordance with the present study.

3. EXPERIMENTAL METHODOLOGY

3.1 Spectroscopy

Spectroscopy is based on quantum mechanics, which is the prevailing theory of the behavior of atoms and molecules. One of the conclusions of quantum mechanics is that the energies of the various forms of motion within atoms and molecules are limited to certain discrete values; that is, they are quantized. When an atomic or molecular system absorbs or emits light, the system goes from one quantized energy level to another. The Bohr frequency condition states that the difference in the energy levels must equal the energy of the light absorbed or emitted. Spectroscopy uses this principle to probe the energy levels of the matter under study. A Perkin Elmer FTIR Spectrometer, available at the Thermal Systems Laboratory (LST-PUCPR) was used for the measurements, and to obtain the spectral reflective data of 3mm thickness clear glass sample.

3.2 Measurements for 3mm Clear Glass

In this section, we present the measurements obtained directly from the FTIR Spectrometer. Fig. 1 shows the frontal reflectance of a sample of 3mm clear glass. The single-surface reflectivity at short wavelengths is less than 0.1 and slowly decreases with increasing wavelength. After dropping to nearly zero at 8 μm, as it is usual in this type of glass, ρ shows two major resonances around 9 and 21 μm, attributable to how silicon oxide stretches and bends when influenced by network modifiers (Sidorov, 1967). The main effect of the chemical differences among this glass occurs in the visible and near-infrared spectra.

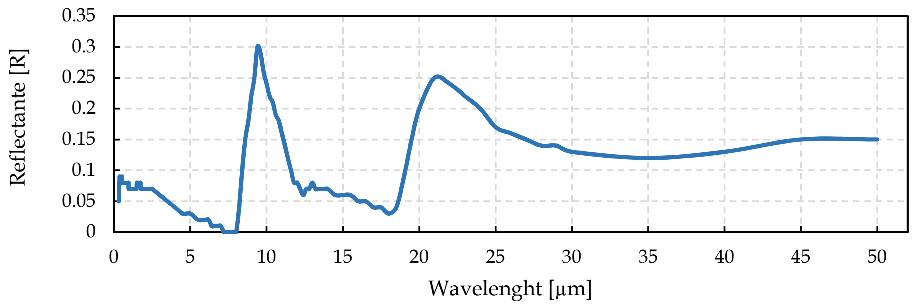

Figure 1. Reflectance Measurements for 3mm Clear Glass

3.3 Partial Results for 3mm Clear Glass

Figure 2 presents the results obtained as solution of Eq. (4). The spectral phase angle data will be used to evaluate the index of refraction (n) and coefficient of extinction (k) yielded by Eq. (2) and Eq. (3) respectively.

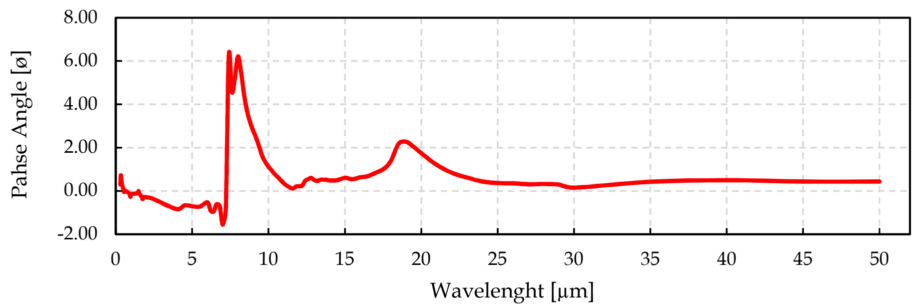

Figure 2. Estimated Phase Angle due Eq. (4)

4. RESULTS

The spectral values for the index of refraction and coefficient of extinction are shown in Fig. 3 and Fig. 4. We may observe a coherent behavior in relation to the index of refraction, with values around 1.5 in the visible spectrum. Figure 4 includes the results for the coefficient of extinction, which varies between 9 - 12 μm and 20 - 25 μm and presents the typical resonance sectors on silica glasses. The results for the index of refraction and coefficient of extinction are compared in the next section, which includes available literature data to verify the computational code to obtain these spectral optical constants using spectral reflectance measurements.

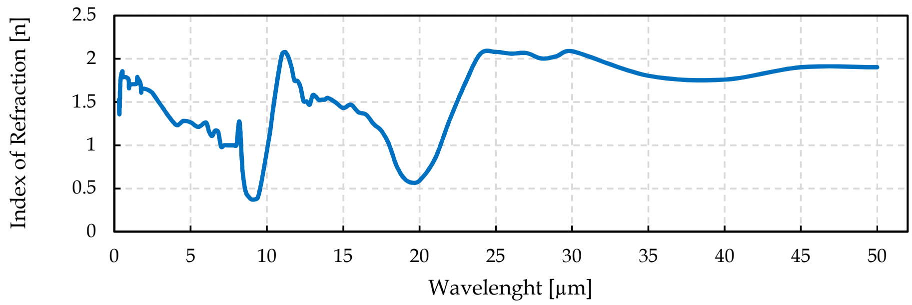

Figure 3. Results for Optics Constants

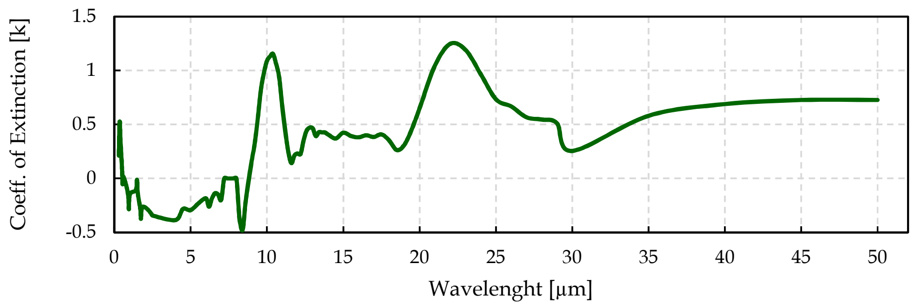

Figure 4. Results for Optics Constants

4.1 Validation of Numerical Integration Model

This section includes the support of classical literature to verify our results, namely Rubin (1985) for soda lime silica glasses and Hsieh and Su (1979) for thermal radiative properties of glass. Figure 5 presents the experimental results on continuous blue (n) and red (k) lines, evidencing the proximity between both results and the aforementioned studies is clear.

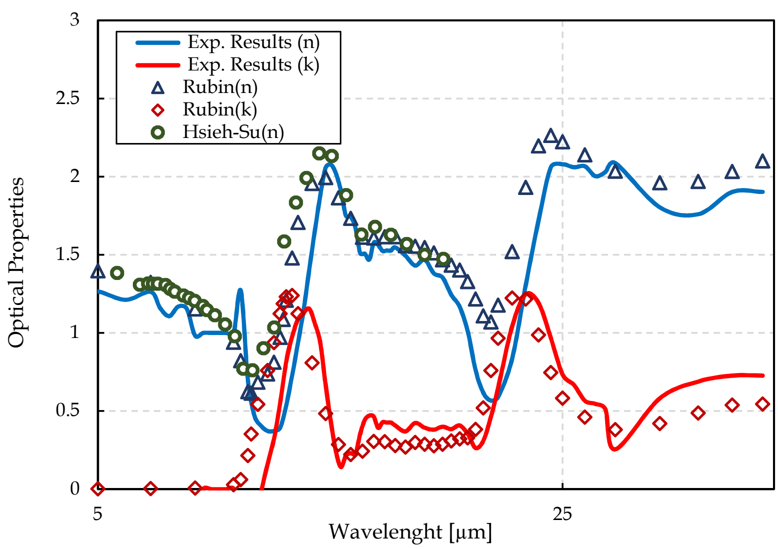

Figure 5. Validated Optics Constants

5. CONCLUSIONS

The real and imaginary parts of the complex index of refraction ($\hat{n} = n + ik$) are essential values to characterize a given material within the electromagnetic spectrum. Knowing the spectral behaviour of the index of refraction allows one to estimate how much energy is transmitted, reflected, and absorbed by the media on different parts of the electromagnetic spectrum. In this article, we presented the results of a computational code that uses numerical integration to obtain the phase angle of the complex index of refraction from measurements of spectral reflectance. Using the model presented by Rubin (1985) with spectral values of phase angle and reflection coefficient is able to determinate the spectral values of the real and imaginary parts of the complex index of refraction. We concluded that the developed algorithm is able to compute the real and imaginary part of the complex index of refraction for silica lime glasses from experimental spectrometry using frontal reflection data of a silica glass sample. The values for n and k were compared with results presented by two different articles (Rubin (1985), Hsieh and Su (1979)) with a very good proximity for results. This work is the initial development of numerical codes to be included in future studies to determine the radiative behavior of thin-film coatings on glass substrates.

6. ACKNOWLEDGEMENTS

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