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Infrared spectra of the main optical properties of polystyrene obtained using the Drude-Lorentz model of complex relative permittivity

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Infrared spectra of the main optical properties of polystyrene obtained using the Drude-Lorentz model of complex relative permittivity

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Abstract

This study investigates whether classical dispersion analysis using the Drude-Lorentz model can effectively and simply derive a comprehensive set of optical properties for polystyrene from its infrared reflection-absorption (IRRA) spectrum and how these derived properties compare with those in the existing literature. The spectra of these properties were derived from the complex relative permittivity using the Drude-Lorentz model for permittivity. The reflection-absorption spectrum of a polystyrene (PS) thin film applied to a metallic mirror was analyzed using classical dispersion techniques. This approach, validated by a strong fit between experimental and modeled spectra, offers a significantly simpler workflow than multistep or computationally intensive techniques and allows the extraction of the main spectra of the optical properties of polystyrene from its reflection-absorption spectrum. This is based on an iterative least-squares fit of the experimental reflection-absorption spectrum of the polymer with the theoretical spectrum derived from the complex permittivity of the Drude-Lorentz model. This method is distinctive in its capability to calculate the complex relative permittivity, from which a wide array of main optical properties are comprehensively derived, such as the complex electrical modulus, energy loss function, optical constants, absorption coefficient, penetration depth, dissipation factor, and complex optical conductivity, all from a single reflection-absorption spectrum measurement, streamlining the characterization workflows. In addition, some optical properties of PS films are discussed, which could be beneficial for the research of polystyrene-based composites and the development of polystyrene copolymers.

Keywords: infrared (IR) spectra, polystyrene (PS), optical properties, classical dispersion analysis, complex relative permittivity, complex electric modulus, energy loss function, optical constants, absorption coefficient, penetration depth, dissipation factor, optical conductivity.

Introduction

The optical properties of polystyrene (PS) in the infrared (IR) spectrum are essential for polymer analysis. While techniques such as Fourier-transform infrared spectroscopy and Kramers-Kronig analysis are frequently used to acquire IR spectra of the optical constants n and k [1-3], they often require specific sample preparations or complex computational steps that limit their applicability for routine analysis of thin films.

In this study, classical dispersion analysis was effectively used to interpret the IR reflection-absorption spectra of PS thin films. Our objective is to demonstrate the ability of this innovative method to easily and accurately determine a comprehensive set of optical properties for PS thin films, including complex permittivity, electric modulus, and optical constants, solely from their IR reflection-absorption spectra. We hypothesize that this approach will provide a comprehensive and reliable characterization of properties such as complex relative permittivity, electric modulus, optical constants, and absorption coefficient, offering a simple yet robust alternative to conventional methods. This innovative method simplifies the determination of the main optical properties of superficial polymer films by directly integrating classical dispersion analysis with reflection-absorption spectroscopy, reducing the need for complex sample preparation or indirect data processing steps often associated with other techniques.

The measured spectrum was a transflection spectrum. The measured dimension was the transmittance. The transflection spectra were similar to the transmission spectra [4-6]. Classical dispersion analysis uses the Drude-Lorentz model of independent oscillators, which describes the complex relative permittivity $\varepsilon(\nu)$ using the following equation:

$$\tilde{\varepsilon}_r(\nu) = \frac{\tilde{\varepsilon}(\nu)}{\varepsilon_0} = \varepsilon_\infty + \sum_j \frac{\nu_{pj}^2}{\nu_{0j}^2 - \nu^2 - i\gamma_j \nu} \quad (1)$$

Each oscillator is represented by a Lorentzian with three adjustable parameters: oscillator frequency $\nu_{0,j}$, linewidth γ_j, and plasma frequency $\nu_{p,j}$. The parameter ε_∞ represents the contributions of higher-frequency oscillators. The parameter ε_0 is the vacuum permittivity (= 8.854×10^{-12} F/m) [7].

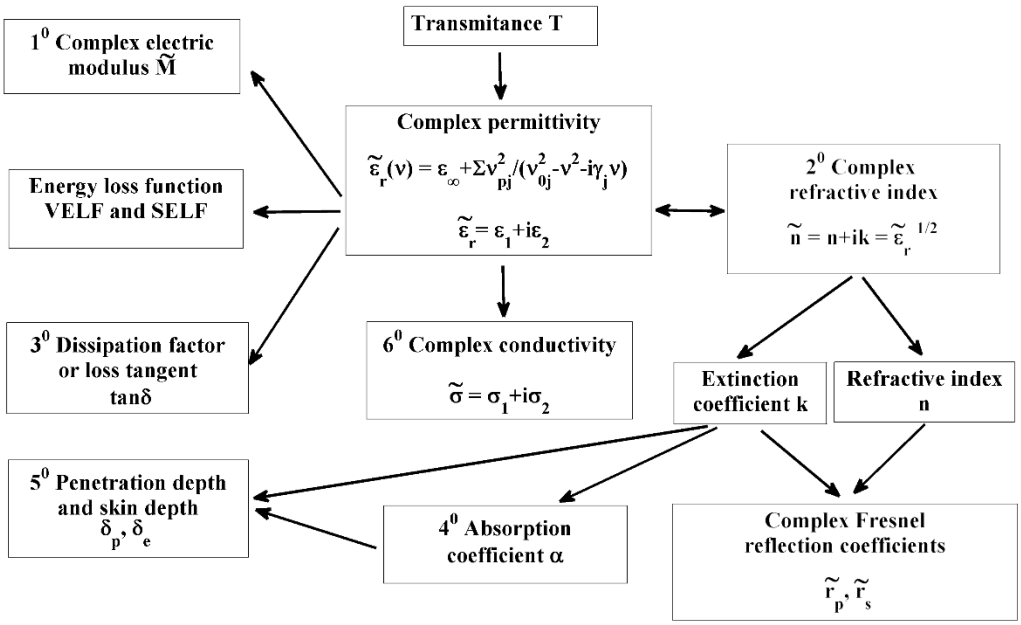
The modeling process consists of introducing the dispersion parameters ε_∞, ν_0, ν_p, and γ, corresponding to the independent oscillators of the different groups in the polymer structure, in the expression of complex relative permittivity described by the Drude-Lorentz equation, and adjusting them until the transmittance T_{model} obtained from the modeled complex relative permittivity approximates the best $T_{experimental}$ transmittance corresponding to the reflection-absorption spectrum of the polymer [4-6, 8].

Complex relative permittivity in Eq. (1) is systematically adjusted by modifying the parameters ε_∞, ν_0, ν_p, and γ until the minimum value of the specified quantity is achieved as follows:

$$\chi^2 = \sum_i^N \left(\frac{y_i - f(\nu_i, p_1 \ldots . p_M)}{\sigma_i} \right)^2 = \chi^2(p_1, \ldots . p_M) \quad (2)$$

The error bars for the experimental data are denoted by σ_i. The chi-square χ^2 is the sum of the squares of the differences divided by σ_i between the experimental and model transmittance values. In this equation, y_i is the value of the experimental transmittance at frequency ν_i. The transmittance of the model with a set of internal parameters (p_1,…. p_M), at the same frequency, are denoted as f(ν_i, p_1,…. p_M). The Levenberg–Marquardt algorithm, also known as the damped least-squares method, was used to solve this problem [7].

Classical dispersion analysis based on the previously presented model (Drude-Lorentz) was used to obtain the complex relative permittivity. This quantity is the basis of Scheme 1.



Scheme.1 Obtaining the main optical properties of the polymer film from the complex permittivity [6].

The novelty of this work lies in the simple method of obtaining infrared (IR) spectra of the main optical properties from the reflection-absorption spectra of thin polymer films, circumventing the complexities or specific sample requirements inherent in other established techniques. They were obtained from the infrared spectra of the

complex relative permittivity obtained by the classical dispersion analysis of the infrared (IR) reflection-absorption spectra of PS thin films. The relationships between them were used. All these quantities depend on the temperature and frequency of the radiation. Thus, the spectra of these quantities were obtained.

Experimental

Thin films of PS were obtained by depositing a solution of the polymer dissolved in chloroform on the surface of the copper metal samples. Atactic polystyrene (with a molecular weight Mw =135 kg/mol and a polydispersity index Mw /Mn = 1.05 from Polymer Source, Inc.) was used as received. A copper metal mirror was chosen as the substrate for the PS film because copper has high reflectance values (1>R>0.99) in the investigated IR spectral range. Thin films were obtained using the drop-casting method. Polymer solutions with concentrations of 0.5–4 g/L were cast by dropping them onto the horizontal surface of the metal mirrors to obtain films with different thicknesses on the order of micrometers [6].Spin-coating techniques [9-12] or dip-coating [13,14] are commonly used to obtain thin films on surfaces. However, they can induce a specific orientation of the polymer chain during the casting of the polymer film. Therefore, we employ an original drop-casting technique [6] to minimize chain orientation, carefully controlling the parameters to achieve uniform thickness. Thus, thin films of controlled and uniform thicknesses are obtained on the entire surface of the metallic mirror [7]. To obtain a thin film with a uniform thickness, we decreased the evaporation rate of the solvent. After evaporation of the solvent, the polymer coated metal sample was kept for 2 h in a vacuum chamber at a pressure of 10^{-1} torr and a temperature of 120 $^{\circ}$C to evaporate the traces of solvent. Although meticulous vacuum drying was used to minimize residual solvents, their potential presence remains a critical factor that can subtly alter the polymer spectrum [15]. The presence of residual solvents can alter the processed spectrum by introducing spurious absorption bands or shifting peak positions. The metal surface used as the substrate for the polymer film was obtained by grinding and polishing the metal.

The infrared reflection-absorption (IRRA) spectrum of the PS thin film was recorded at a 20 ° incidence angle within the spectral range of 500-4000 cm^{-1}, at a resolution of 2 cm^{-1} using the specular reflectance device of the Carl Zeiss Jena UR-20 spectrophotometer. The experimental error bar for the measured IRRA spectrum is 0.01.

The free RefFIT calculation program was used to obtain the dielectric function and theoretical spectrum of the PS film based on the Drude-Lorentz model by applying a classical dispersion analysis [16]. The theoretical spectrum was fitted to the experimentally measured spectrum by continuously adjusting the model parameters. A thin film with a thickness of 1.6 μm was achieved. Because incident radiation crossed the polymer film twice after reflection on the metal mirror, a thickness of 0.8 μm was used. The thickness obtained corresponds to the concentration of the polymer in the chloroform solution. A set of 14 damped harmonic oscillators was empirically determined to provide the best fit to the experimental spectrum, balancing the complexity of the model with precision, and was used to fit the polymer model spectrum to the experimental spectrum digitized at 1659 experimental points.

Results and Discussions

The IRRA spectrum of the thin PS film deposited on a copper mirror was processed using the RefFIT calculation program, which uses classical dispersion analysis based on the Drude-Lorentz model, according to relation (1) [7]. Figure 1 shows the mid-infrared range of 500-4000 cm^{-1} of the two PS thin film spectra: the experimental

reflectance-absorption spectrum and the model transmission spectrum based on the Drude-Lorentz equation (1).

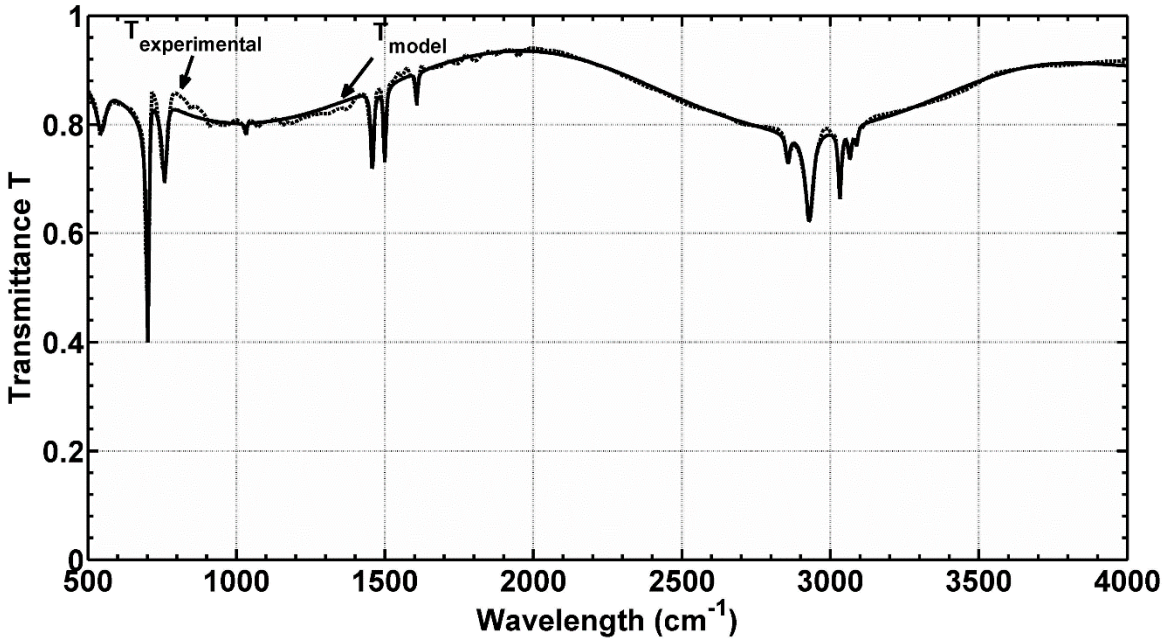


Fig. 1 Comparison of the experimental IR reflection-absorption spectrum $T_{experimental}$ with the transmission model spectrum T_{model} obtained by classical dispersion analysis with the RefFIT program, for PS film

A good match between the two spectra was observed over the entire analyzed spectral domain, with a chi-square value of 956.304 for 1569 experimental points, indicating a strong fit.

The complex relative permittivity $\tilde{\varepsilon}_r$

The complex relative permittivity and thickness of the thin film of PS deposited from a chloroform solution on the surface of a copper mirror were obtained by fitting the Drude-Lorentz model of complex relative permittivity with that of the experimental reflection-absorption spectrum. A good fit was observed for the model constructed using the experimental spectrum.

The IR spectra of the real and imaginary parts of the complex relative permittivity of a PS film deposited from solutions on a metallic steel mirror are presented in Figure 2. A value of 1.6 μm for the thin film was obtained by fitting the data to the model.

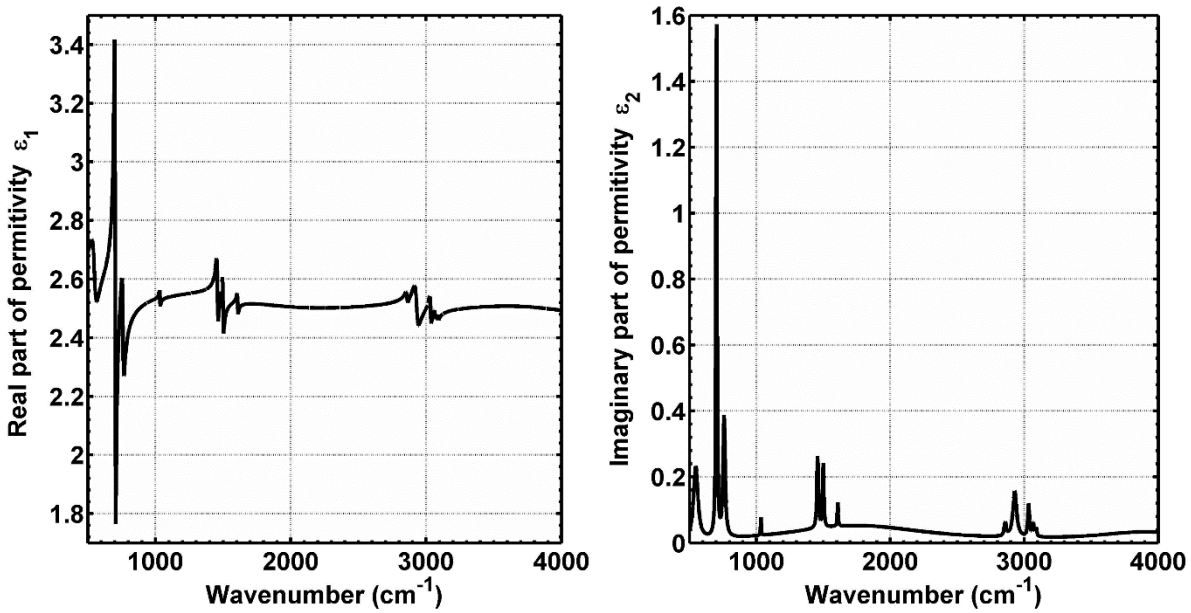


Fig. 2 IR spectra of the real part ε_1 and respective the imaginary part ε_2 of the complex relative permittivity for the thin PS film cast on a copper mirror

The complex electric modulus $\widetilde{M}$

The reciprocal of the complex relative permittivity is the complex electric modulus [17, 18]. This provides a clearer characterization of dipolar relaxation mechanisms in polymeric films. Equation (3) defines the complex electric modulus,

$$\widetilde{M} = \frac{1}{\widetilde{\varepsilon}_r} = M_1 + iM_2 = \frac{\varepsilon_1}{\varepsilon_1^2 + \varepsilon_2^2} + i\frac{\varepsilon_2}{\varepsilon_1^2 + \varepsilon_2^2}. \quad (3)$$

Figure 3 shows the real and imaginary parts of the complex electric modulus, expressed in relation (3).

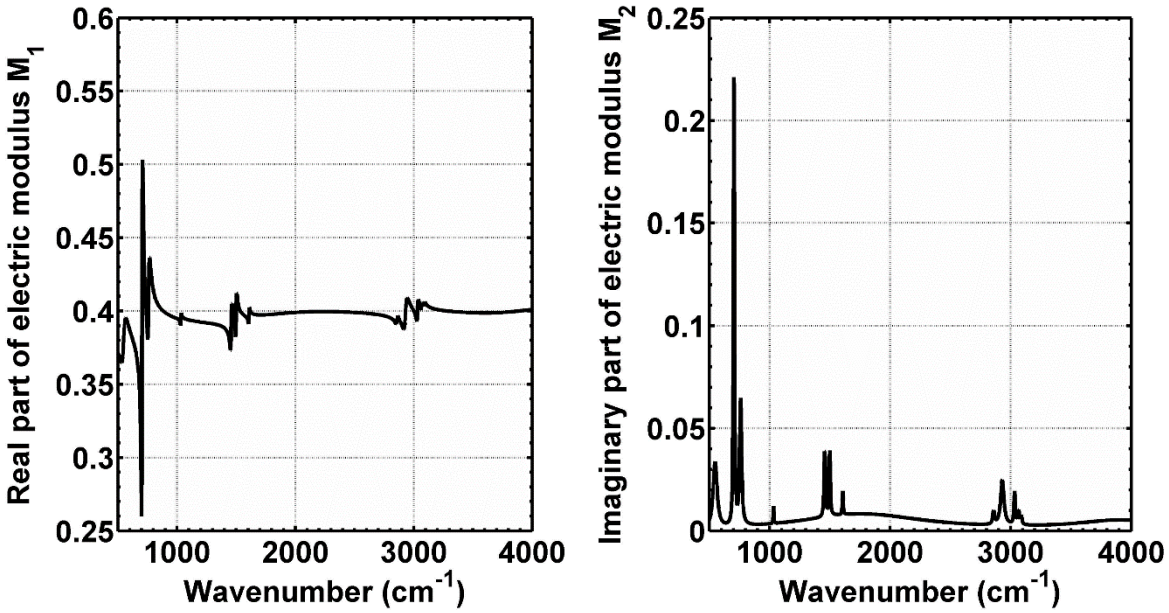


Fig. 3 IR spectra of the real part M_1 and the imaginary part M_2 of the complex electric modulus of the thin PS film cast on a copper mirror

The IR spectra of the real and imaginary parts of the complex relative permittivity and complex electric modulus were similar.

The imaginary part of the complex electric modulus M_2 was calculated in the RefFIT program [16] as a loss function L_f, or defined as a volume energy-loss function (VELF) [19-21]. The energy-loss function (ELF) describes the energy lost while passing through a film. The ELF has two main sections: surface energy-loss function (SELF) and VELF. The ELF is the sum of two quantities, both obtained from ε_1 and ε_2. The real part ε_1 refers to dispersion and ε_2 refers to the absorption of light waves in an optical medium. The two ELF terms are given by the following relations:

$$\begin{aligned} M_2 = \mathrm{VELF} = \mathrm{Im}\left(-\frac{1}{\tilde{\varepsilon}_r}\right) = \frac{\varepsilon_2}{\varepsilon_1^2+\varepsilon_2^2} = L_f; \\ \mathrm{SELF} = \mathrm{Im}\left(-\frac{1}{\tilde{\varepsilon}_r}+1\right) = \frac{\varepsilon_2}{\left(\varepsilon_1^2+1\right)^2+\varepsilon_2^2}. \end{aligned} \tag{4}$$

The two components of the ELF are defined by Eq. (4) are presented in Figure 4 for the PS film cast on the copper mirror. The VELF described by El-Nahass et al. [19] is the same as the imaginary part M_2 of the complex electric modulus and the loss function L_f defined by Kuzmenko [16]. SELF describes the inelastic reflection of electrons on the flat surface of a solid without considering spatial dispersion. SELF represents the energy loss of free charge carriers when they traverse the surface of a material [21]. The ratio of the two components of the energy loss function, VELF/SELF, is presented in Figure 4. In the spectral regions where the thin film exhibited high absorption, high values of this ratio were obtained.

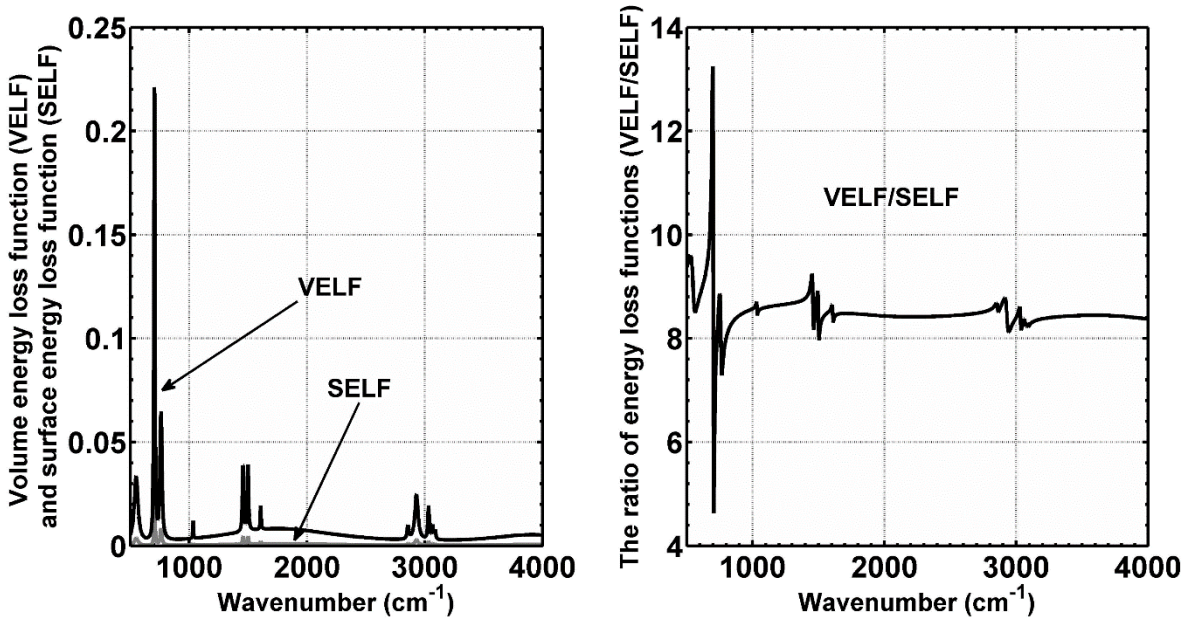


Fig. 4 IR spectra of the energy loss functions (ELF) and the ratio of the two components volume energy loss function (VELF) and surface energy loss function (SELF) for the PS film cast on the copper mirror

The complex refractive index $\tilde{n}$

This was obtained from the complex relative permittivity using the following equation:

$$\tilde{n} = n + ik = \sqrt{\tilde{\varepsilon}_r}. \tag{5}$$

The refractive index n, which is the real part of the complex refractive index, describes the dispersive properties of the materials. It can be calculated from the complex permittivity [22, 23].

$$n = \mathrm{Re}\left(\tilde{\varepsilon}_r\right) = \sqrt{\frac{1}{2}\left(\sqrt{\varepsilon_1^2 + \varepsilon_2^2} + \varepsilon_1\right)}. \tag{6}$$

The extinction coefficient k is the imaginary part of the complex refractive index that describes the absorbing properties of the material and can be calculated from the complex permittivity using the following equation:

$$k = \mathrm{Im}\left(\tilde{\varepsilon}_r\right) = \sqrt{\frac{1}{2}\left(\sqrt{\varepsilon_1^2 - \varepsilon_2^2} - \varepsilon_1\right)} = \frac{\varepsilon_2}{2n}. \tag{7}$$

The refractive index n and extinction coefficient k spectra were obtained from the complex relative permittivity based on Equations (5-7). Figure 5 shows the IR spectra of the refractive index n and the extinction coefficient k of the PS film cast on a metal mirror.

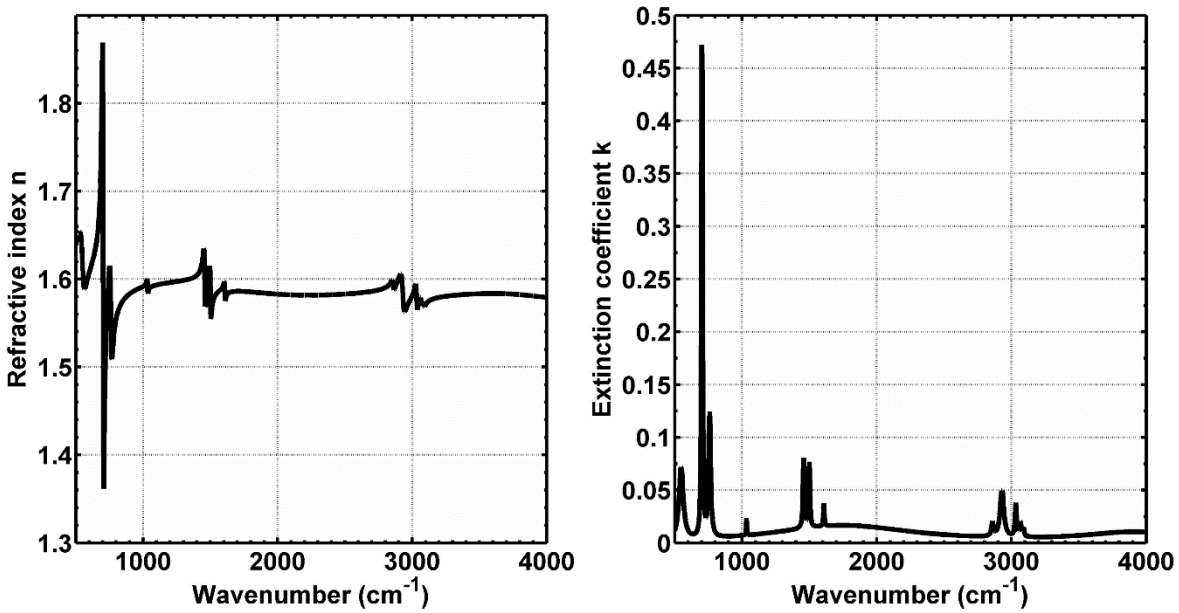


Fig. 5 IR refractive index n and extinction coefficient k spectra of the PS film cast on a copper mirror

Similar data have been obtained by other authors by processing the ATR-IR or transmission spectra [24, 25]. Other authors have studied PS films using Kramers-Kronig analysis of the specular reflection spectra [26] or by interpreting spectroscopic ellipsometry measurements [27].

The dissipation factor (or dielectric loss tangent) tan δ

The amount of energy dissipated inside a polymer when interaction with an electromagnetic wave can be described by the dissipation factor or the dielectric loss tangent (tan δ). The loss tangent, tan δ, was used to investigate the ability of a material to absorb an electromagnetic field [17, 18, 21, 28]. It is defined as the ratio of the imaginary part to the real part of the complex relative permittivity.

$$\tan\delta = \frac{\varepsilon_2}{\varepsilon_1}. \tag{8}$$

Figure 6 shows the IR spectrum of the dissipation factor tan δ of the PS film cast on a metal mirror.

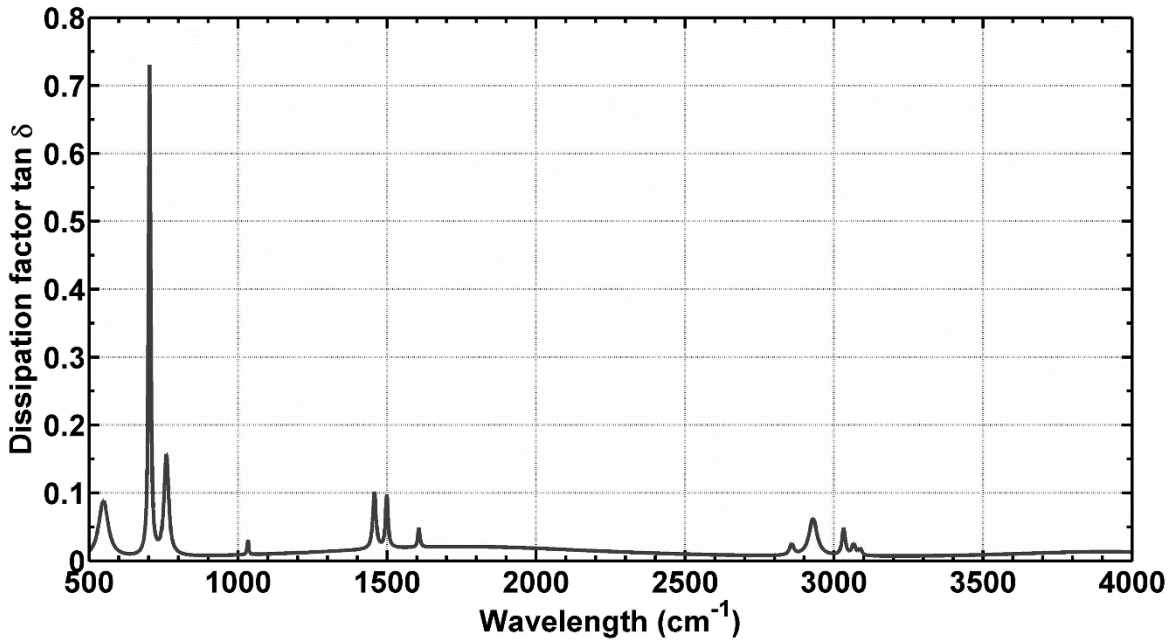


Fig. 6 IR spectrum of the dissipation factor tan δ of the PS) film cast on the copper mirror

This spectrum is similar to that of the imaginary part ε_2 of the complex permittivity.

The absorption coefficient α

The absorption coefficient was obtained using the extinction coefficients. This allow us to measure the amount of light absorbed by the material. [19-21, 29-33].

$$\alpha = \frac{4\pi}{\lambda} k = 2\frac{\omega}{c} k. \tag{9}$$

The absorption coefficient α, expressed by relation (9), is proportional to the extinction coefficient k and the radiation frequency. Therefore, the absorption bands at high frequencies are expected to be more intense than those in the extinction coefficient spectrum. The change in the appearance of the absorption band at 3400 cm^{-1} is better highlighted. Figure 7 shows the IR spectrum of the absorption coefficient, α.

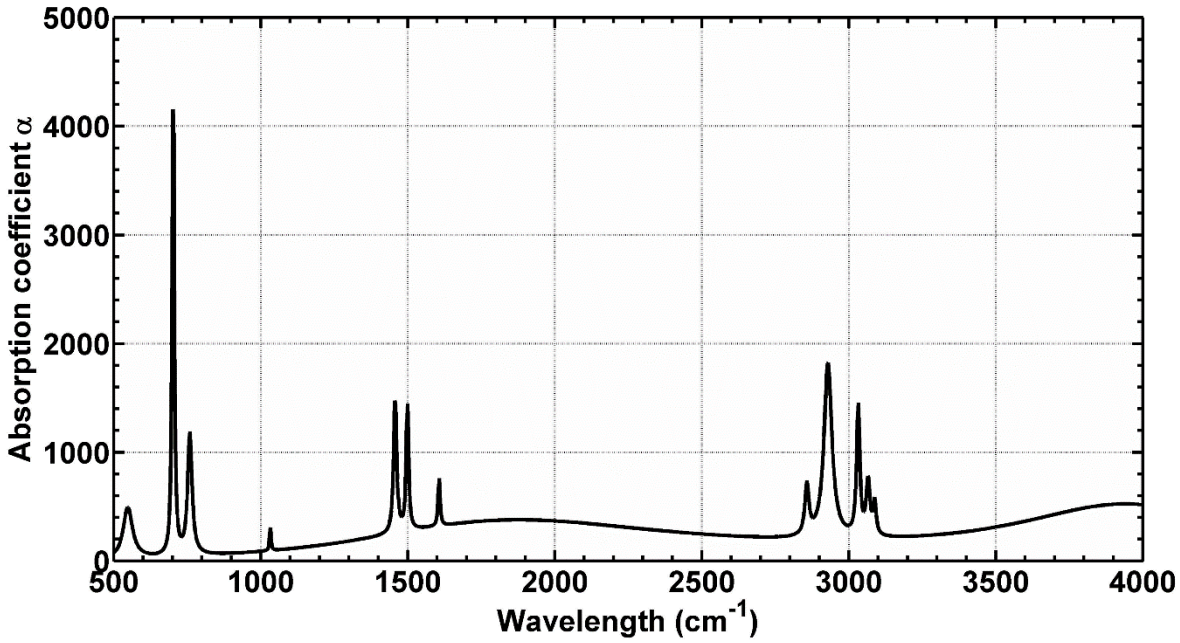


Fig. 7 IR spectrum of the absorption coefficient of the PS thin film cast on a copper mirror, obtained by classical dispersion analysis of the reflection-absorption spectrum with the RefFIT program

Penetration depth δ_p *and skin depth* δ_e.

When radiation is reflected on a surface that separates two different media, part of the radiation is reflected, and the other part is absorbed in the medium in which it is refracted. The penetration depth is defined as the depth at which the intensity or power of the field within the material decays to 1/e of the surface value [34]. Skin depth δ_e is the depth at which the intensity of the electric field decreases to 1/e of its value at the surface of the material.

$$\delta_p = \frac{1}{\alpha} = \frac{\lambda}{4\pi k} \quad ; \quad \delta_e = \frac{2}{\alpha} = 2\delta_p \tag{10}$$

The penetration depth has an IR spectrum that differs from that of other optical properties. Figure 8 shows the IR spectrum of the penetration depth of the PS film cast on a metal mirror.

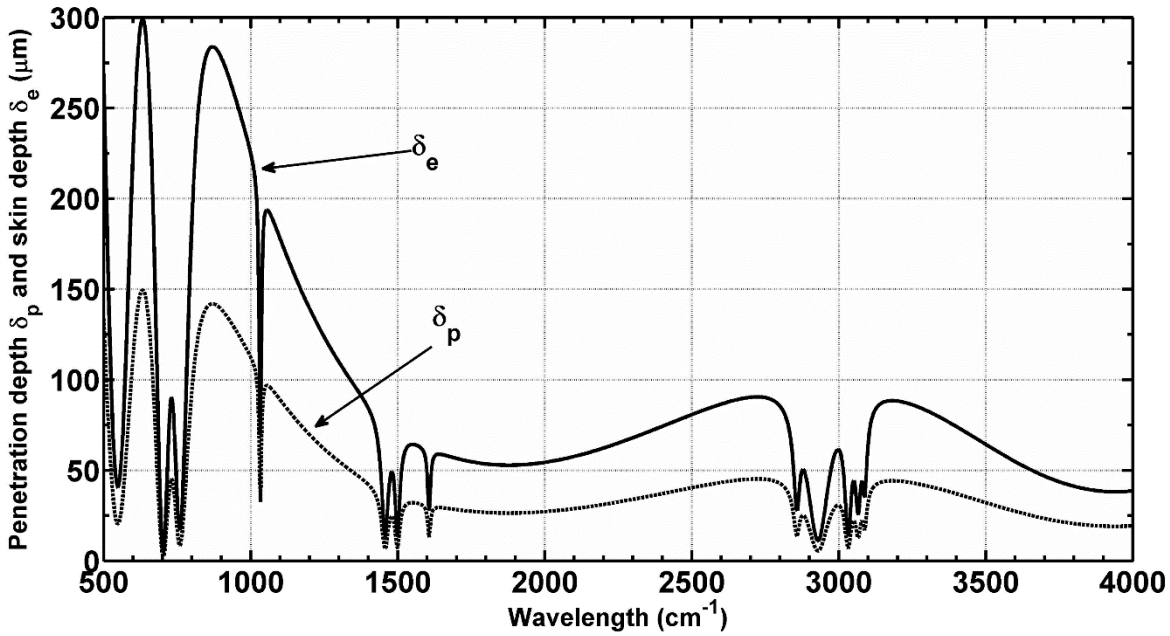


Fig. 8 IR spectrum of the penetration depth δ_p of the radiation through the thin PS film, cast on a copper mirror

It can be seen that in the spectral regions where the film has the highest absorption, the penetration depth of radiation through the thin film decreases much and the absorption process is limited near the surface [34]. The penetration depth was greater than the thickness of the thin film (1.6 μm) in almost all spectral regions. Radiation refracted at the air-film interface can reach the polymer-metal interface and is reflected on the metallic mirror (with a high reflectance coefficient R_{23}=0.894) [4]. During some processes of thermal degradation or as a result of polymer irradiation, the reflection-absorption spectrum decreases significantly, so that a spectrum of reflection-absorption is no longer obtained, but instead, a spectrum of specular reflection is obtained.

Complex optical conductivity $\tilde{\sigma}$

Complex optical conductivity measures the response of a material to light and is related to complex relative permittivity [19-21, 32, 35-37]. Complex permittivity describes the extent of electron displacement when a field is applied, whereas complex conductivity describes the speed of electron movement under the influence of the applied field. The complex optical conductivity provides details regarding the structural and optoelectronic properties of a material.

The imaginary part of the complex permittivity $\varepsilon_{2,}$ which determines the absorption of the wave inside the medium, contributes to the real part of the optical conductivity. The real part of the complex permittivity $\varepsilon_{1,}$ which expresses the dispersive properties of the medium, contributes to the imaginary part of the optical conductivity.

$$\tilde{\varepsilon} = \varepsilon_0 \tilde{\varepsilon}_r = \varepsilon_0 \left(\varepsilon_1 + i\varepsilon_2\right) = \varepsilon_0 + \frac{i\sigma}{\omega} = \varepsilon_0 \left(1 + \frac{i\sigma}{\varepsilon_0 \omega}\right). \tag{11}$$

$$\sigma_1 = \varepsilon_0 \omega \varepsilon_2; \sigma_2 = \varepsilon_0 \omega \varepsilon_1. \tag{12}$$

where ω is the angular frequency (rad/s).

There are subtleties in the calculation of the optical conductivity. Some authors [37-39] calculated the real part of the optical conductivity in the CGS system of units using the following equation:

$$\sigma_{opt}(\mathrm{CGS}) = \frac{nc\alpha}{4\pi}. \tag{13}$$

To obtain the conductivity value in the International System of Units (SI), the previous equation must be multiplied by $4\pi\varepsilon_0$ [40].

$$\sigma_{opt}(\mathrm{SI}) = 4\pi\varepsilon_0\sigma_{opt}(\mathrm{CGS}) = 4\pi\varepsilon_0\frac{nc\alpha}{4\pi} = nc\alpha\varepsilon_0 = \varepsilon_0\omega\varepsilon_2. \tag{14}$$

or else:

$$\begin{aligned}\sigma_{opt}(\mathrm{SI}) &= \frac{1}{9\cdot10^9}\sigma_{opt}(\mathrm{CGS}),\\ \sigma_{opt}(\Omega^{-1}\mathrm{m}^{-1}) &= \frac{1}{9\cdot10^9}\sigma_{opt}(\mathrm{s}^{-1}).\end{aligned} \tag{15}$$

The IR spectra of the real part σ_1 and the imaginary part σ_2 of the optical conductivity of the PS film cast on the metal mirror are shown in Figure 9.

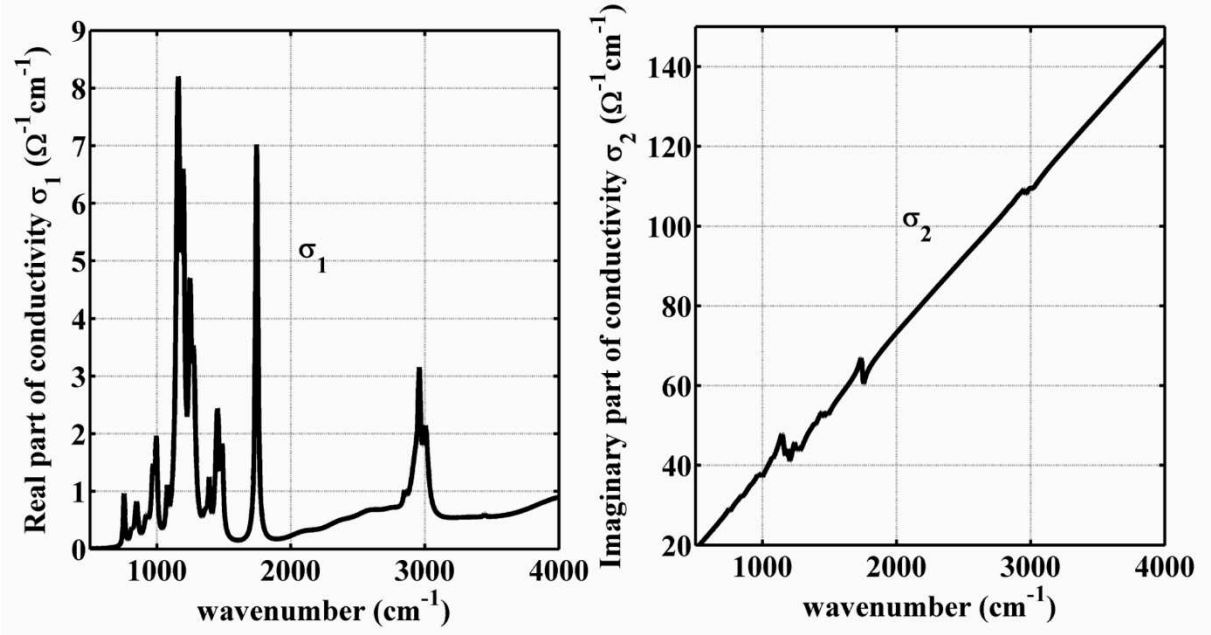


Fig. 9 IR spectra of the real part σ_1 and the imaginary part σ_2 of the optical conductivity for the thin PS film cast on a copper mirror

The real part of the conductivity contains the same information as the imaginary part of the dielectric function. Therefore, their IR spectra were similar to each other. The optical conductivity σ_{opt} is less significant for simple polymers with dielectric properties than for complex polymers. It is used mainly in the case of conductive polymers, called organic metal polymers, or in the case of semiconductor materials, to detect the allowed inter-band optical transitions.

The optical properties of PS (ε_2, M_2, VELF, SELF, k, α, tan δ, and σ_1), which depend directly on the absorbing properties of the polymer, present similar IR spectra. The optical properties (ε_1, M_1, and n) that depend on the dispersion of radiation in the medium through which it passes also exibit similar IR spectra.

Limitations

Although this study provides a robust method for determining the optical properties, certain limitations should be noted. The accuracy of the Drude-Lorentz model is based on the correct assignment of damped harmonic oscillators, and variations in the fitting parameters can influence the derived properties.

Although meticulous vacuum drying was used to minimize residual solvents, their potential presence remains a critical factor that can subtly alter the polymer spectrum [6]. The presence of residual solvents can alter the processed spectrum by introducing spurious absorption bands or changing peak positions. Future work could include more rigorous in situ monitoring of solvent evaporation and quantitative analysis of the effects of residual solvents on optical properties.

A significant limitation arises during processes such as thermal degradation or polymer irradiation, where the reflection-absorption spectrum can decrease significantly, potentially transitioning to a specular reflection spectrum. In such cases, classical dispersion analysis might yield distorted or inaccurate optical properties, as the underlying assumptions of the reflection-absorption model are violated. Researchers should be cautious when applying this method to degraded or irradiated samples and consider complementary techniques to verify spectral integrity.

A key limitation for accurate analysis is encountered when the penetration depth (δp) is less than the thickness of the thin film. In such spectral regions, the radiation does not fully traverse the film to be reflected from the metallic mirror, leading to specular reflection rather than transflection. This can severely distort the derived optical properties, rendering the information inaccurate and unreliable. It could also lead to misinterpretation of material properties or erroneous conclusions about polymer behavior. Researchers employing this technique must carefully consider the thickness of the film in relation to δp, especially in highly absorbing regions, and potentially adjust sample preparation or utilize alternative methods for such conditions. Penetration depth analysis revealed spectral regions in which the film thickness might exceed the penetration depth, potentially leading to distorted spectra owing to specular reflection. Future work could explore the impact of film inhomogeneity or surface roughness, which were not explicitly addressed in this study.

Conclusions

The significance and novelty of this work lie in the simple, demonstrated approach to determine the complex relative permittivity and subsequently obtain the main optical properties of PS, as evidenced by the consistent spectral derivations presented in this study. Classical dispersion analysis and the Drude-Lorentz model were used to process the IRRA spectra of the polymer. The IR spectra of the real and imaginary parts of the complex relative permittivity were used to obtain the spectra of the main optical properties of PS.

The analysis revealed that several derived optical properties (k, α, $\sigma 1$, M2, SELF, and tan δ) exhibited IR spectra similar to the imaginary part of the complex permittivity $\varepsilon 2$, while others (n and M1) mirrored the real part $\varepsilon 1$. This consistency underscores the robust interrelationships between these properties and suggests that tracking key indicators, such as the refractive index n and the extinction coefficient k, is sufficient for monitoring polymer transformations.

A critical consideration for an accurate analysis is the relationship between the penetration depth and the film thickness. As shown in Figure 8, the penetration depth exceeded the film thickness in most spectral regions. In such cases, if the thickness of the film is greater than δp, true transflection may not occur, and specular reflection can distort the spectrum, potentially leading to inaccurate optical properties.

In spectral regions where the thin film exhibited high absorption, large VELF/SELF ratios were obtained.

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