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► **To cite this version:**

J. Bichon, A. Pillet, A. Sklia, D. Petitprez, Romain Peretti, et al.. Complex refractive index determination of PTFE, TPX and polypropylene windows for TeraHertz broadband spectroscopy. 2022 47th International Conference on Infrared, Millimeter and Terahertz Waves (IRMMW-THz), Aug 2022, Delft, Netherlands. pp.1-2, 10.1109/IRMMW-THz50927.2022.9895520 . hal-03794330

HAL Id: hal-03794330

<https://hal.science/hal-03794330v1>

Submitted on 6 Oct 2022

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Complex refractive index determination of PTFE, TPX and polypropylene windows for TeraHertz broadband spectroscopy

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Abstract—We perform TeraHertz characterization of three low-loss polymer candidates, i.e. polytetrafluoroethylene, polymethylpentene, and polypropylene, to choose the material with the proper opto-mechanical properties for aerosol and gas broadband spectroscopy cell windows. Samples are analyzed with the TeraHertz time domain spectroscopy technique. Then, the time-traces are fitted with theoretical models and the real and imaginary parts of their complex refractive indices are extracted using the Fit@TDS algorithm developed by Photonic TeraHertz team members.

I. INTRODUCTION

POLYMERS are valuable materials in research for their exceptional properties such as durability and resistance. They are, for instance, widely used in optical assemblies as lenses or windows due to their transparency in the visible and TeraHertz (THz) range. However, only few studies have calculated their complex refractive indices (CRI) and data from 3 to 10 THz is almost non-existent [1].

Broadband spectroscopy in the THz is of paramount importance in the study of aerosols and/or gases to understand current issues such as climate change [2] or disease diagnosis [3]. Nonetheless, the analytical equipment needs windows with opto-mechanical requirements (e.g. withstanding pressure, avoiding degassing and maximizing transmission). A complete optical characterization of the deployed materials in optical assemblies is therefore essential before taking measurements.

In this regard, three low-loss polymer candidates, i.e. polytetrafluoroethylene (PTFE – 2.5 mm thick), polymethylpentene (TPX – 2 mm) and polypropylene (PP – 50 microns), are analyzed with a TeraHertz Time Domain Spectrometer (THz-TDS – TDS Terasmart from Menlo systems, 90 fs/1.5 μ m laser; 850 ps delay line). In comparison with other techniques, THz-TDS has the advantage of measuring the time-dependent amplitude $E(t)$ and hence simultaneously acquiring the amplitude and the phase. There is therefore no need of empirical models or Kramers-Kronig analysis to get the CRI [4].

The real and imaginary parts of the CRI are extracted from the time-traces and fitted with theoretical models using the Fit@TDS software developed by THz Photonic team members at IEMN [5]. For nonpolar polymers, the model used is the Lorentz oscillator. The fit is based on 4 parameters: the permittivity, and the resonance frequency, the linewidth, and the strength of the oscillator for each oscillator [6]. An extrapolation is carried out for PTFE (beyond 5 THz) and for PP (beyond 7.3 THz).

II. RESULTS

The CRI of PTFE from 0.2 to 8 THz are reported in the figures below (Fig.1). The figures show a Lorentz-shaped resonant absorption at 0.91 THz with a linewidth of 0.12 THz above a broad band of higher frequency. Our results demonstrate a broad absorption band of small oscillator strength characteristic of low-loss polymers at 2.48 THz. These two resonances can be attributed to weak lattice modes. An intense Lorentz oscillator absorption peak is at 5.71 THz. This peak is found by extrapolation and corresponds to the twisting mode of CF₂. Previous studies indicate only a broad absorption band in the measured range and confirm the intense peak around 6 THz. These results go beyond previous reports by showing the presence of a weak absorption peak at 0.91 THz thanks to a better signal/noise ratio [7,8].

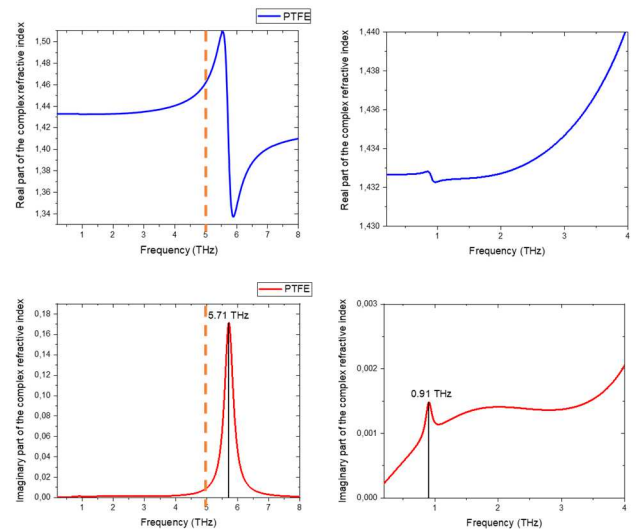


Fig. 1. The real (blue) and imaginary (red) parts of the CRI of PTFE from 0.2 to 8 THz on the left. On the right, a zoom between 0.2 and 4 THz. The results indicate 3 Lorentz oscillator resonance at 0.91, 2.48 and 5.71 THz. The extrapolation was performed in the range after the orange dotted line.

PP exhibits 3 Lorentzian shape absorption peaks at 2.32, 5.19 and 7.56 THz (Fig.2). Similarly, the two weak peaks can be assigned to lattices modes and the one at 7.56 THz is probably due to CH vibrations. A comparable conclusion was reached by reported findings regarding the frequencies of the resonances [9]. Although the intensity of the peak at 7.56 THz is clearly higher than that of the two other absorptions as in our case, the precision of the measurements in the literature does not allow to compare the intensities of the peaks.

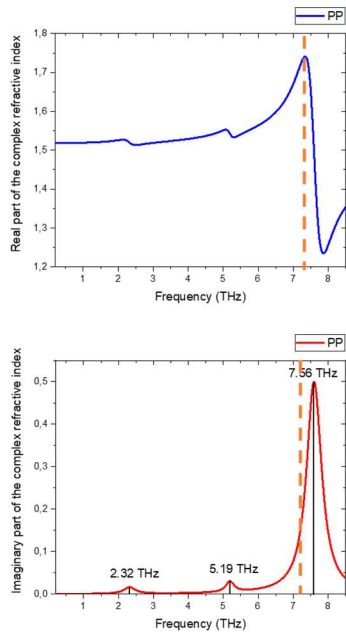


Fig. 2. The real (blue) and imaginary (red) parts of the CRI of PP from 0.2 to 8.5 THz, showing 3 Lorentz shape resonance at 2.32, 5.19 and 7.56 THz. The extrapolation was performed in the range after the orange dotted line.

TPX has a wide absorption band at 3.56 THz of low oscillator strength due to lattice mode vibrations (Fig.3). The variations of the real and imaginary parts are of the order of 10^{-3} in the measurement frequencies range. Furthermore, the TPX has no absorption peak from 0.2 to 5 THz that could interfere with measurements. Nevertheless, further studies should be carried out to study its behavior beyond 5 THz.

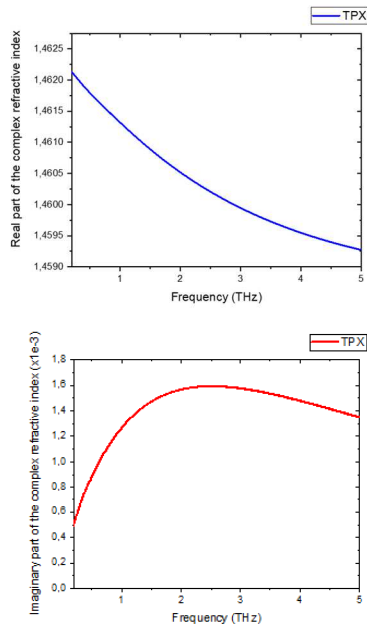


Fig. 3. The real (blue) and imaginary (red) parts of the CRI of TPX from 0.2 to 5 THz. TPX has a singular weak and broad absorption band at 3.56 THz with a linewidth of 38.3 THz.

III. SUMMARY

This study adds to a corpus of research showing the dielectric properties of non-polar polymers in the THz range. Collectively, our results appear to be consistent with those in the literature. However, our measurements show a better resolution at low frequency and a better signal-to-noise ratio. Additionally, more than 8 THz is reached in some cases, while most studies have results that stop at around 3 THz. During the conference, an overview of the dielectric, optical and mechanical properties of the three materials will be provided during the conference to enable proper comparison and benchmark of the windows.

IV. ACKNOWLEDGMENT

The authors gratefully acknowledge the financial support of the French National Research Agency (ANR-20-CE42-0002 STEPSON). The authors also appreciated the support by the CaPPA project (Chemical and Physical Properties of the Atmosphere) funded by the French National Research Agency (ANR) through the PIA (Programme d'Investissement d'Avenir) under contract « ANR-11-LABX-0005-01 ».

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