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An impact of multiple wave reflections in a flat sample on material parameter reconstruction using THz pulsed spectroscopy

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Abstract. The present paper is dedicated to studying the accuracy of sample material parameter reconstruction using terahertz (THz) pulsed spectroscopy. The technique for characterizing the material parameters of thin flat samples allowing to take into account multiple wave reflections in a flat have been considered. While transmitting through the resonant sample, THz pulse undergoes multiple reflections, which result in satellite pulses in THz waveform. The accuracy of material parameter reconstruction strongly depends on the number of satellite pulses. We have analytically estimated an impact of satellite pulses on material parameter reconstruction by considering the local linearization of theoretical sample transfer function based on the model of quasi-Fabry-Perot-resonator.

1. Introduction

Terahertz (THz) pulsed spectroscopy (TPS) appeared in 1975 as a result of Auston's research of semiconductor photoconductivity under the femtosecond optical pumping [1]. Since the emergence of highly stable portable femtosecond lasers TPS becomes a powerful tool for fundamental and applied research. TPS provides an ability both for sample material parameter reconstruction [2–12] and for studying the internal structure of the sample (T-Ray tomography) [13–15].

Regardless the type of data we are measuring the main principle of TPS operation could be formulated as follows. THz pulse is generated with one of the existing techniques [1,16–19], and the electric field of THz pulse is detected [20] with a high time resolution after the transmission of pulse through the sample or after the reflection of pulse from its surface. By applying a fast Fourier transform to time-domain data, it is possible to analyze the complex transmission and reflection coefficients of the sample [12], in a wide frequency range, as well as to study the sample pulse response [13,14]. All the specified characteristics form an initial conditions for TPS inverse problem solutions. There are many applications for TPS systems, including condensed matter spectroscopy [21], gas sensing [22], spectroscopy of colloid crystals [23], protein crystals [24–26], medical diagnosis [27–36], security task [37–39] etc. Recently, TPS has become a useful tool for nondestructive evaluation of polymer composite constructions [40–42].

Owing to the wide variety of TPS applications, many TPS signal processing problems appear, for instance, the inverse scattering problems. Reconstructing the resonant sample material


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parameters in transmission mode is a representative example of TPS inverse problem [2–12]. Most TPS inverse problems, regardless the specificity of reconstructed data, are ill-posed, and the accuracy of reconstruction depends on a large number of factors [11,12]. The stability of the TPS inverse problem solution in presence of different factors must be systematically studied for correct implementation of TPS signal processing.

In this paper, we present new results for sample material parameter reconstruction using TPS. We are analyzing a commonly used algorithm for resonant sample material parameter reconstruction based on quasi-Fabry-Perot model, which takes into account THz pulse transmission through the resonance sample [7,10,12]. While transmitting through the resonant sample THz pulse undergoes multiple reflections, thus, the THz waveform contain finite number of satellite THz pulses. Depending on the number of these satellite pulses we could obtain different reconstruction accuracy. We are estimating the impact of satellite pulse number on the accuracy of material parameter reconstruction utilizing the local linearization of quasi-Fabry-Perot model.

2. Quasi-Fabry-Perot approach for material parameter reconstruction

At first, let us describe a common material parameter reconstruction procedure [7,10,12], which we are considering in the present paper. This technique helps to reconstruct the complex refractive index of the flat homogeneous sample

$$\widetilde{n}\left(\nu\right)=n'\left(\nu\right)-in''\left(\nu\right)=n'\left(\nu\right)-i\frac{\alpha\left(\nu\right)c_0}{2\pi\nu}, \tag{1}$$

where ν is a frequency of electromagnetic wave, c_0 is a speed of light in vacuum, $n'(\nu)$ and $n''(\nu)$ are real and imaginary parts of complex refractive index, and $\alpha(\nu)$ is an absorption coefficient. The technique we are describing is appropriate for studying the resonant flat samples, transparent in THz frequency range and having the thickness

$$l>l_{min}=\frac{c_0}{\nu_{max}n_{min}}, \tag{2}$$

where n_{min} is the minimal value of sample refractive index within the range of system sensitivity, $[\nu_{min},\nu_{max}]$.

Reconstruction of sample material parameters, $\widetilde{n}_1$, is produced by minimization of the following error functional

$$\widetilde{n}_1\left(\nu\right)=\mathrm{argmin}_{\widetilde{n}_1(\nu)}\Big[M\left(\nu,\widetilde{n}_1\right)+A\left(\nu,\widetilde{n}_1\right)\Big], \tag{3}$$

where

$$M\left(\nu,\widetilde{n}_1\right)=\left|\left|\widetilde{H}_{exp}\left(\nu\right)\right|-\left|\widetilde{H}_{th}\big(\nu,\widetilde{n}_1\big)\right|\right|^2,\qquad A\left(\nu,\widetilde{n}_1\right)=\left|\phi\left[\widetilde{H}_{exp}\left(\nu\right)\right]-\phi\left[\widetilde{H}_{th}\big(\nu,\widetilde{n}_1\big)\right]\right|^2, \tag{4}$$

$\widetilde{H}_{exp}(\nu)$ and $\widetilde{H}_{th}(\nu,\widetilde{n}_1)$ correspond to experimental and theoretical transfer functions of the sample, $|...|$ and $\phi[...]$ represent estimation of transfer function modulus and phase.

Functional minimization (equation (3)) could be implemented separately for different Fourier-domain frequencies ν. The details of functional minimization process are described in paper [12]. The experimental complex transfer function $\widetilde{H}_{exp}(\nu)$ can be calculated using the relation

$$\widetilde{H}_{exp}\left(\nu\right)=\frac{\widetilde{E}_s\left(\nu\right)}{\widetilde{E}_r\left(\nu\right)}, \tag{5}$$

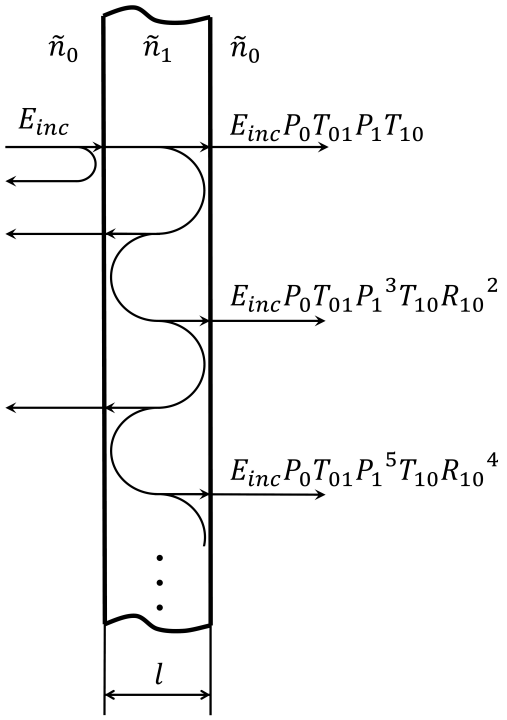


Figure 1. Schematic representation of multiple light scattering in the flat.

where tildes stand for Fourier transform, $\widetilde{E}_r(\nu) = F_t^{-1}[E_r(t)]$ and $\widetilde{E}_s(\nu) = F_t^{-1}[E_s(t)]$, of reference and sample waveforms, $E_r(t)$ and $E_s(t)$. Theoretical transfer function is based on the quasi-Fabry-Perot model [12] of the wave propagation through the sample (figure 1):

$$\widetilde{H}_{th}(\nu, \widetilde{n}_1) = \frac{4\widetilde{n}_0\widetilde{n}_1}{(\widetilde{n}_0 + \widetilde{n}_1)^2} exp\left(-ik\left(\widetilde{n}_1 - \widetilde{n}_0\right) l\right) \left[1 + \sum_{\xi=1}^{k} \left(\frac{\widetilde{n}_0 - \widetilde{n}_1}{\widetilde{n}_0 + \widetilde{n}_1} exp\left(-ik\widetilde{n}_1 l\right)\right)^{2\xi}\right], \quad (6)$$

where k represents the number of satellite pulses in sample waveform, $E_s(t)$, l is a thickness of sample, and $\widetilde{n}_0$ is a refractive index of air. This equation is based on the Bouguer-Lambert law, describing wave propagation through dissipative medial, as well as on the Fresnel equations for light reflection and transmission through the interface of two media (we are utilizing Fresnel formulas for the case of normal light incidence on the surface of interface).

The sample waveform contains a limited number of satellite pulses, k, owing to the finiteness of the TPS time-domain window [12]. Therefore, a finite number of pulses should be taken into account during the $\widetilde{n}_1(\nu_t)$ computation. k can be easy calculated during the TPS waveform pre-processing $E_s(t)$ [7,10,12]. Obviously, the accuracy of material parameter reconstruction strongly depends on k. We are estimating this dependence by means of local linearization of sample transfer function model (6).

3. Local linearization of theoretical transfer function

Many factors impact the material parameter reconstruction accuracy, including the noises in TPS waveforms and fluctuations of various TPS parameters. Studying these factors is very important for correct implementation of TPS measurements [12]. All factors lead to appearance

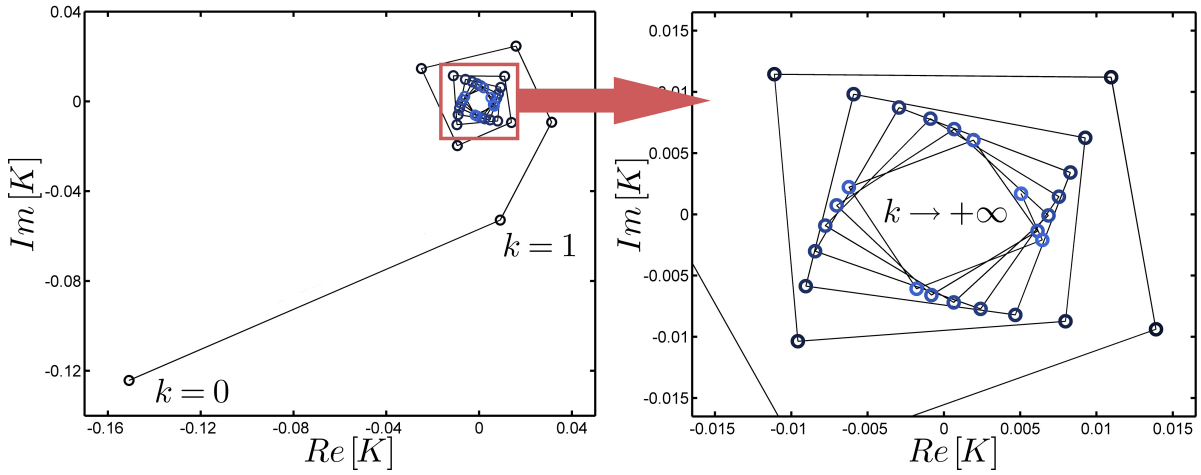


Figure 2. Local linearization of quasi-Fabry-Perot model: **(a)** shows K for all possible numbers of multiple resonances within the sample, $k = 0, 1, 2, ..., +\infty$, and **(b)** shown magnified part of complex plane centered near the zero-point and marked with red box in (a) panel.

of an error in TPS waveforms, ΔE, and, as a consequence, to appearance of an error in transfer function, $\Delta\widetilde{H}$. The latter one usually varies with frequency variations, $\Delta\widetilde{H} = \Delta\widetilde{H}(\nu)$, and it leads to appearance of an error in reconstructed material parameters, $\Delta\widetilde{n}_1 = \Delta\widetilde{n}_1(\nu)$.

We are estimating an impact of transfer function error, $\Delta\widetilde{H}$, on material parameter reconstruction error, $\Delta\widetilde{n}_1$, for different number of satellite pulses, k. Rigorous relation between $\Delta\widetilde{n}_1$ and $\Delta\widetilde{H}$ is defined by quasi-Fabry-Perot model (6), and it has a complex character in case $k > 0$. Therefore, we perform local linearization of (6)

$$\Delta\widetilde{n}_1(\nu) = K\Delta\widetilde{H}(\nu), \tag{7}$$

where K is a coefficient of local linearization depending on the condition of experiment, $K = K(\nu, k, l, \widetilde{n}_0, \widetilde{n}_1)$. We have calculated K for a certain experimental conditions ($\widetilde{n}_0 = 1.0$, $\widetilde{n}_1 = 2.00 + i0.477$, $\nu = 1.0$ THz, and $l = 0.1$ mm) and for various number of satellite pulses, k, in a sample signal, thus, the dependence $K(k)$ have been obtained. Figure 2 shows the results of $K(k)$ calculations.

With an increase of k the modulus of local linearization coefficients, $|K(k)|$, decays. Thus, the more satellite pulses we are detecting and taking into account during material parameter reconstruction, the higher reconstruction accuracy we could achieve for a certain power of noises in TPS waveforms, $E_r(t)$ and $E_s(t)$. Moreover, $K(k)$ dependence oscillates around zero point, $(0, 0)$, of complex plane with an increase of k, therefore, the relation between the impact of transfer function error on real and imaginary parts, n' and n'', of material parameters differs for various number of satellite pulses. Simplest techniques for material parameter reconstruction allow reconstructing $\widetilde{n}_1$ using only main pulse of the sample waveform, while satellite pulses are being canceled by means of window filtering. Obviously, neglecting the satellite pulses could significantly reduce the computation complexity. At the same time it could strongly reduce the accuracy of material parameter reconstruction, as follows from figure 2.

4. Conclusion

We have studied the technique for material parameter reconstruction using TPS allowing to take into account multiple pulse reflection in a flat homogeneous sample. We have estimated an impact of the satellite pulses on the accuracy of material parameter reconstruction by

applying the local linearization to the sample model which has the form of quasi-Fabry-Perot resonator. Strong dependence of the material parameter error on the number of satellite pulses has been observed. We have demonstrated that the average error of material parameter reconstruction reduces with an increase of satellite pulses number, thus, the more pulses we could detect with particular time-domain window of TPS, the higher accuracy of material parameter reconstruction we could achieve.

Acknowledgments

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