A Comparison of Terahertz Pulsed Spectroscopy and Backward-Wave Oscillator Spectroscopy

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Abstract. This paper presents new experimental and theoretical results for the material parameter reconstruction utilizing the terahertz (THz) pulsed spectroscopy (TPS). The material parameter reconstruction algorithm was realized and experimentally implemented to study the test sample. The algorithm takes into account multiple reflections of THz pulse within the flat sample during the transmission mode measurements. Therefore the samples with small thickness or low refractive index could be studied utilizing the proposed method. In order to estimate the reconstruction accuracy, test sample material parameters, obtained with the TPS, were compared with the results of the same sample studying by the use of the backward-wave oscillator (BWO) spectroscopy. Thus, high reconstruction accuracy was demonstrated.

1. Introduction
Terahertz (THz) pulsed spectroscopy (TPS) is proved to be a convenient instrument for characterizing materials in THz frequency range [1]. TPS utilizes short pulses of THz radiation with a wideband spectrum in frequency-domain to measure the THz spectral material parameters [2–4] or to study the internal structure of the sample [5]. TPS signal processing and TPS inverse ill-posed problem solution are important for various fields of physics. In TPS, the electric field of the THz pulse is detected with a high time resolution after the transmission of a pulse through the sample or after the reflection of a pulse from the surface. By applying a fast Fourier transform to the measured THz waveforms, it is possible to analyze the complex transmission or reflection coefficients of the sample in a wide frequency range. Depending on the techniques, utilized for the THz pulse generation and detection, the reliable frequency range of TPS operation could cover different ranges of the electromagnetic spectrum.

There are many applications for THz technology and, in particular, TPS systems. The list of applications includes spectroscopy of semiconductors [6], gas sensing [7], security task [8–10], and medical diagnosis (diagnosis of skin cancers [11–13], skin burns [14,15], breast tumors [16], cancer of colonic tissue [17], etc.). Recently, TPS has become a useful tool for the nondestructive evaluation of polymer constructional materials and composite structures [18,19].

In this paper, the new experimental and theoretical results for the material parameter reconstruction using TPS system are presented and discussed. A common material parameter
reconstruction technique [2–4] is realized and experimentally implemented for studying the test sample optical properties. In order to both verify the material parameter reconstruction procedure and to estimate the reconstruction accuracy, obtained material parameters of the test samples are compared with the results of the same samples studying by the use of the backward-wave oscillator (BWO) spectroscopy [20–23].

2. Materials and Methods

The conventional TPS system [5, 24], which is based on the generation of THz pulses in PC antenna and detection of THz waveforms using electro-optical sampling, is used. The TPS system works in transmission mode allowing determination of the sample complex transmission coefficient in the frequency range between 0.1 and 3.0 THz.

A common material parameter reconstruction procedure, which is similar to the one described in papers [2–4], is used as the basis for the material parameter reconstruction. This technique helps to determine the spectral complex refractive index \( \tilde{n}_1(\nu_t) \) of the flat sample on the basis of the experimental sample complex transfer function \( \tilde{H}_{\text{exp}}(\nu_t) \). Note, multiple reflections of THz radiation within the flat sample, leading to the appearance of the satellite THz pulse in TPS waveforms, are considered [4]. Thus, flat samples with small thickness and low refractive index could be studied.

The sample thickness \( t \) needs to be measured before the TPS waveform processing with an accuracy better than 0.05 mm. Considering the typical measurement conditions, the flat samples, which are transparent in the THz frequency range and have a thickness greater than 100–200 \( \mu \)m, could be studied. The list of important conditions for correct algorithm implementation also includes height sample flatness, sample homogeneity, and small roughness of the sample surface. The maximal angle deviation between the flat surface normal and the axes of the THz beam should be smaller than 5° [2].

Material parameter reconstruction is produced by means of the error functional \( \Phi(\nu_t, \tilde{n}_1(\nu_t)) \) minimization:

\[
\tilde{n}_1(\nu_t) = \arg \min_{\tilde{n}_1(\nu_t)} \left[ \Phi(\nu_t, \tilde{n}_1(\nu_t)) \right] = \arg \min_{\tilde{n}_1(\nu_t)} \left[ M(\nu_t, \tilde{n}_1(\nu_t)) + A(\nu_t, \tilde{n}_1(\nu_t)) \right],
\]

where \( M(\nu_t, \tilde{n}(\nu_t)) \) and \( A(\nu_t, \tilde{n}(\nu_t)) \) depend on the experimental \( \tilde{H}_{\text{exp}}(\nu_t) \) and theoretical \( \tilde{H}_{\text{th}}(\nu_t, \tilde{n}(\nu_t)) \) transfer functions of the flat sample

\[
M(\nu_t, \tilde{n}_1(\nu_t)) = \left| \tilde{H}_{\text{exp}}(\nu_t) - \tilde{H}_{\text{th}}(\nu_t, \tilde{n}_1(\nu_t)) \right|^2,
\]

\[
A(\nu_t, \tilde{n}_1(\nu_t)) = \left| \phi \tilde{H}_{\text{exp}}(\nu_t) - \phi \tilde{H}_{\text{th}}(\nu_t, \tilde{n}_1(\nu_t)) \right|^2.
\]

where \( [...] \) and \( \phi [...] \) represent the modulus and the phase of the complex functions, respectively.

Functional minimization (Eq. (1)) could be implemented separately for different frequencies \( \nu_t \) of the discrete Fourier-domain. Beginning at a certain \( \nu_t' \) which corresponds to the highest TPS sensitivity, we can calculate the sample complex refractive index \( \tilde{n}_1(\nu_t') \) and use it as an initial assumption for the neighboring \( \tilde{n}_1(\nu_t + \Delta \nu_t) \) computation, where \( \Delta \nu_t \) is a step of the discrete Fourier-domain. This approach for \( \Phi(\nu_t, \tilde{n}_1(\nu_t)) \) minimization excludes an appearance of non-physical breaks in reconstructed material parameter curves.

The experimental complex transfer function \( \tilde{H}_{\text{exp}}(\nu_t) \) can be measured using the relation

\[
\tilde{H}_{\text{exp}}(\nu_t) = \frac{\tilde{E}_s(\nu_t)}{\tilde{E}_r(\nu_t)},
\]
Lambert law is

\[ T_{ij} = E_{i}^{-1} [E_{r,i}(t)] \]

defined by the Fresnel relations. The wave propagation through the medium along the distance \( E \) satellite pulses in the sample waveform \( E_{s}(t) \). where \( N \) represents the number of multiple THz pulse reflection within the flat (number of satellite pulses in sample waveform \( E_{s}(t) \)). In (4), the complex operator \( \tilde{P}_{ij} (\nu, \nu_{t}) \) describing the wave propagation through the medium along the distance \( z \) and defined by the Bouguer-Lambert law is

\[
\tilde{P}_{ij} (\nu, \nu_{t}) = \exp (-i2\pi \tilde{n}_{\nu_{t}}(\nu_{t})z),
\]

\( \tilde{T}_{ij} \) and \( \tilde{R}_{ij} \) in (4) are complex operators describing the transmission and the reflection of the THz pulse at the interface between the i-th and j-th media and defined by the Fresnel relations

\[
\tilde{T}_{ij} (\nu_{t}) = \frac{2\tilde{n}_{i}(\nu_{t})}{\tilde{n}_{i}(\nu_{t}) + \tilde{n}_{j}(\nu_{t})}, \quad \tilde{R}_{ij} (\nu_{t}) = \frac{\tilde{n}_{j}(\nu_{t}) - \tilde{n}_{i}(\nu_{t})}{\tilde{n}_{i}(\nu_{t}) + \tilde{n}_{j}(\nu_{t})}.
\]

The sample waveform contains a limited number of satellite pulses \( N \) owing to the finiteness of the TPS time-domain window; therefore, a finite number of pulses should be taken into account during the \( \tilde{n}_{1}(\nu_{t}) \) computations. An effective sample thickness correction, based on criterion of the material parameter curve smoothness [2, 4], is applied during the material parameter reconstruction to increase the measurement accuracy.

3. Material Parameter Reconstructed with TPS and BWO spectroscopy

BWO spectroscopy is a very precise tool for determining material parameters at the GHz and THz frequencies. It has attracted an extensive amount of research on the methodology of dielectric measurements with BWO spectroscopy [21–23, 25]. However, BWO spectroscopy suffers from a limited sensitivity range \( (\nu_{t} \leq 1.4 \text{ THz}) \) and relative measurement complexity compared to the TPS. As such, the material characterization in a wide frequency range is produced using a set of BWO sources because the reliable spectral range of each BWO is limited to \( \leq 100 \text{...200 GHz} \). In addition, two sample and reference signals must be obtained to correctly reconstruct a sample complex refractive index using a BWO system. Conversely, TPS spectroscopy requires only one reference and sample waveform to obtain the complex transfer function of sample in a wide frequency range. Therefore, to determine the sample material parameters, TPS appears to be more convenient.

In order to compare TPS with the BWO spectroscopy techniques, several test samples were studied. The described TPS system as well as BWO spectrometer based on a Golay-cell detector were used for this purpose. Figure 1 shows the results of the test sample material parameter reconstruction: (a) shows the refractive indexes \( n_{1}(\nu_{t}) \) and (b) shows the absorption coefficients \( \alpha_{1}(\nu_{t}) \) of the test samples. The following three flats were studied: (1) is a highly absorbing \( 0.46 \text{ mm} \) thick ceramic sample, (2) is a GaAs 1.19 mm thick flat, and (3) is a low-absorbing 1.37 mm thick sample. The described algorithm was implemented for the TPS waveforms processing, and the standard BWO spectroscopy data technique [21–23] was utilized. Continuous curves in Fig. 1 represent the TPS measurements, and the markers show the BWO spectroscopy results. Furthermore, the error bars indicate a \( \pm 3\% \) uncertainty for the BWO spectroscopy measurements.
Figure 1. Comparison of the test-sample material parameters obtained with TPS and BWO spectroscopy: (a) shows the refractive indexes and (b) shows the absorption coefficients of (1) highly absorbing 0.46 mm-thick ceramic flat, (2) 1.19 mm-thick GaAs flat, and (3) low-absorbing 1.37 mm-thick ceramic flat.

One could note high accuracy of the material parameter reconstruction, since the TPS measurements results match the confidence interval of the BWO measurements. Accurate reconstruction was demonstrated for both high-absorbing (Fig. 1, curves 1) and low-absorbing (Fig. 1, curves 2) flats as well as for cases of satellite pulse appearance in the TPS waveforms (Fig. 1, curves 2 and 3).

4. Conclusion
Novel results for the sample material parameter reconstruction using the TPS are demonstrated in the present work. Material parameter reconstruction procedure allowing studying the flat samples with small thickness or low refractive index, was realized and experimentally implemented for the test sample studying. Comparison of the reconstructed data with the result of the same sample studying by the use of the BWO spectroscopy helps both to verify the algorithm and to demonstrate the accuracy of the proposed technique.

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