ESKİŞEHİR TECHNICAL UNIVERSITY JOURNAL OF SCIENCE AND TECHNOLOGY
A- APPLIED SCIENCES AND ENGINEERING

2024, 25(1), pp. 36-43, DOI: 10.18038/estubtda.1257999

RESEARCH ARTICLE

DERIVATION OF EXPRESSION FOR PHOTOCURRENT DENSITY FOR NON-DESTRUCTIVE TESTING OF 3D PRINTING FILAMENT BY MEANS OF TERAHERTZ SPECTROSCOPY

Iurii KHOROSHAILO [1], Nataliia ZAICHENKO [2], Olga ZAICHENKO [1,*]

[1] Department of Design and Operation of Electronic Devices, Faculty of Automatics and Computerized Technolohies, Kharkiv National University of Radioelectronics, Kharkiv, Ukraine
[2] Department of Microelectronics, Electronic Devices and Appliances, Faculty of Electronic and Biomedical Engineering, Kharkiv National University of Radioelectronics, Kharkiv, Ukraine

This report presents a revised expression for the photocurrent density in terahertz spectroscopy, which is a non-destructive testing technique of particular interest to the authors in the context of 3D printed parts. 3D printing, also known as additive manufacturing, involves creating three-dimensional objects based on computer-aided design (CAD) models. The process entails depositing, joining, or solidifying material under computer control, layer by layer.

Defects in 3D printing, such as weak infill, gaps in thin walls, inconsistent extrusion, layer separation, and bed drop, can lead to low printing quality and render some printed parts unfit and unsafe for use. Moreover, the ability to tamper with internal layers without altering the exterior could result in the production of maliciously defective parts without detection. Therefore, it is crucial to test 3D printed details and filaments at each stage of processing using non-destructive methods.

A comprehensive review of the relevant literature indicates the potential for enhancing measurement accuracy through various improvements in terahertz spectrometer models. The mathematical model for the photocurrent involves a convolution integral of the current density and the laser radiation pulse that irradiates the surface of the material under study. The expression within the integral incorporates parameters such as the duration of the optical pulse, carrier lifetime, and momentum relaxation time. By evaluating the integral, the result can be obtained as two terms, each being a product of an exponent and a complementary error function with the same parameters mentioned earlier.

The calculation involves several steps, including a change of variables during integration. Verification using Maple software demonstrates agreement with analytical calculations and suggests a pathway for further refinement of the expression for the photocurrent density. The Maple program influenced the results by means of repeating same calculation with aid of computer and allowing to compare if analytical results are same and true, also it could be use for simulation and example calculation, for results graphical representation.

The connection between the obtained mathematical expression and its relation to 3D printing (additive manufacturing) exists. The explanation is in that the 3D printer uses filament, filament has defects, defectoscopy of filament in the terahertz domain have models and methods. The research of defectoscopy models and methods is helpful to increase accuracy of measurement of filament defect parameters and account on it and improve the quality of 3D printed details.

Keywords: 3D-filament, Testing, Terahertz, Spectroscopy, Model

1. INTRODUCTION

This report focuses on non-destructive testing methods for evaluating the quality of filaments used in 3D printing. 3D printing, or additive manufacturing, involves constructing three-dimensional objects from CAD models using various processes that deposit, join, or solidify material under computer

*Corresponding Author:olha.zaichenko@nure.ua
Received: 28.02.2023 Published:28.03.2024

control, layer by layer. Filaments for 3D printing are thermoplastic polymers that melt when heated and are extruded through a nozzle to create the desired object.

Defects in 3D printing, such as weak infill, gaps in thin walls, inconsistent extrusion, layer separation, splitting, and bed drop, can result in substandard print quality and render printed parts unsuitable and unsafe for use. Additionally, the ability to manipulate internal layers without affecting the external appearance raises concerns about the potential production of maliciously defective parts without detection. Therefore, it is essential to test both the 3D printed details and the 3D printing filament at every stage of the process, preferably using non-destructive methods.

Several non-destructive testing methods exist, including radiography, ultrasound, and others. Mechanical tests and light microscopy, although standardized, are mostly performed offline, meaning they are time-consuming and destructive. Recent developments have aimed to bring testing closer to the manufacturing process through in-line and on-line measurements, such as the pressure filter test, ultrasonic testing, and spectroscopic monitoring, particularly in the near-infrared (NIR) frequency range. However, each method is limited to specific applications. The pressure filter test lacks reliability with higher additive concentrations and is unsuitable for fibrous materials. Ultrasonic testing is only suitable for low spatial resolution applications, while NIR offers high resolution but is primarily useful for near-surface analysis or thin samples due to its decreasing penetration depth with increasing frequency.

In the following sections, we will demonstrate that terahertz time-domain spectroscopy (THz TDS) in the frequency range between 100 GHz and a few THz holds promise as a non-destructive testing technique for polymeric compounds. THz TDS combines the advantages of high penetration depth, similar to microwaves, with submillimeter spatial resolution. It enables the extraction of frequency-dependent refractive index and absorption coefficient by capturing phase and amplitude information of the propagated electromagnetic wave.

Among the various non-destructive testing methods for polymers, terahertz spectroscopy was chosen due to its wide spectral coverage in the terahertz region, high dynamic range, ability to detect both amplitude and phase, picosecond time resolution, and potential use as a terahertz pump source.

After early work [5,7] there was rapid development of THz TDS. The modern publication are mainly about application so still there are many interesting aspects in the theory.

Terahertz Time Domain Spectroscopy (THz-TDS) has witnessed a surge in popularity in recent decades owing to its broad frequency range and high signal-to-noise ratio. Researchers have devoted substantial efforts to various aspects of this field, encompassing the development of spectroscopy for acquiring high-resolution signals and extracting crucial information from both gas molecules and biological samples.

The study [11] focuses on leveraging the potent THZ-TDS technique for quantitative information extraction. The investigation highlights the estimation of spectroscopy sensitivity by measuring sample concentrations. There was demonstrate this approach through a physical model applied to solid and gas samples. Despite the prevalent use of convolutional mathematical models for enhanced precision, limited attention has been given to measuring uncertainties in the parameters derived from these models.

In this research, author delve into visualizing uncertainties in the optical parameters of a lactose sample, extracted through the Lorentz model of electronic dispersion. This visualization is achieved by numerically evaluating the Hessian matrix, representing second-order partial derivatives of the function at optimized parameters. Subsequently, standard deviations are computed by extracting the diagonal elements of the inverse of the Hessian matrix. These uncertainties are depicted through error bars on the real and imaginary parts of the refractive index of the lactose sample[11].

Simultaneous compensation of lateral and temporal walk-offs between the fundamental wave and the second harmonic wave plays a pivotal role in our homemade air plasma system, resulting in a notable threefold enhancement in THz conversion efficiency. Furthermore, we optimize the efficiency of second harmonic generation for THz radiation. The incorporation of a dual-wavelength half-waveplate contributes to achieving a high THz conversion efficiency exceeding 0.06% at an 800 nm excitation in a dry air environment. This corresponds to an overall enhancement factor of 6.

In the detection phase, there was experimentally explored electro-optic sampling and air-biased coherent detection. Leveraging our air plasma system, we successfully identify two characteristic peaks (4.85 and 5.8 THz) in the rust sample. This underscores the effectiveness of our approach in both enhancing THz conversion efficiency and enabling precise detection of characteristic features in materials [12].

Terahertz time-domain spectroscopy (THz-TDS) has emerged as a potent and versatile tool across various scientific domains, including imaging, material characterization, and layer thickness measurements. Despite its significant success in research settings, the widespread commercialization of this technology has been impeded by the high cost and cumbersome nature of most systems. The primary contributors to the size and expense of these systems are the laser and the optical delay unit (ODU).

In response to these challenges, the efforts was dedicated to the development of THz-TDS systems centered around compact monolithic mode-locked laser diodes (MLLDs). The ultra-high repetition rate (UHRR) of the MLLD is advantageous, enabling the use of shorter ODUs, thereby reducing the overall size and cost of our systems. However, achieving the necessary precision in the ODU to obtain accurate terahertz time-domain signals remains a critical consideration.

To address this challenge, the interferometric extension was introduced and enhanced for UHRR-THz-TDS systems. This extension is characterized by its affordability, compact design, and ease of integration. In this article, we detail the system setup, the extension itself, and the algorithmic procedure for reconstructing the delay axis based on the interferometric reference signal. Our evaluation, based on a dataset comprising 10,000 signal traces, reveals a low standard deviation of the measured terahertz phase at 1.6 THz, as low as 3 mrad.

Additionally, the remaining peak-to-peak jitter of only 20 fs and a record-high peak signal-to-noise ratio of 133 dB at 100 GHz after averaging. The method outlined in this paper not only simplifies the construction of THz-TDS systems but also reduces bulk and cost. Consequently, it facilitates the transition of terahertz technologies from laboratory settings to practical field applications [13].

The critical literature review show versatility of research direction, its relevance. At the same time it forced us to go back to the beginning in order to go through the evolution of scientific thought through personal experience.

The objective of this study is to validate the accuracy of the mathematical calculations in the model THz of [1-3], as they form the foundation for further research in this field.

2. DERIVATION OF EXPRESSION FOR PHOTOCURRENT DENSITY

The photocurrent density in the emitter corresponds to the convolution of the temporal shapes of the exiting optical pulse and of the impulse current response of the photo switch

$$j_{em}(t) = P_{opt}(t) \otimes \left[n_{em}(t) q \upsilon_{em}(t) \right], \tag{1}$$

where $\otimes$ denotes convolution product, $P_{opt}(t)$ is the optical power, are respectively, the charge, density and the velocity of photocarriers on emitting antenna. The current density $n_{em}(t)q\upsilon_{em}(t)$ represents the impulse response of the photo switch, i.e. response to a delta Dirac optical excitation.
We make the assumption that the temporal profile of the optical pulse is Gaussian. Moreover, to get a simple expression for the current, the free-carrier relaxation in both emitting and receiving photo switches is assumed to be governed by a single exponential decay law [3].

We suppose here that the switch is uniformly illuminated and that the bias field E_{DC} is constant over the whole illuminated region. We get the expression of the photocurrent density in the emitter [1, p.64]

$$I_{pc}(t) \approx \mu_e E_{DC} I_{opt}^0 \int_0^{+\infty} \mathrm{e}^{-(t-t')/\tau_p^2 - t'/\tau_c} \left[1 - e^{-t'/\tau_s}\right] dt' = I_1 + I_2 \tag{2}$$

where μ_e is electron mobility, $\mu_e = e\tau_s / m$, m is effective mass of carrier,
E_{DC} is the DC bias field, I_{opt}^0 is magnitude of optic pulse, τ_p is optic pulse duration, τ_c is currier life time, τ_s is momentum relaxation time, I_1 is first term, $I_1 = \mu_e E_{DC} I_{opt}^0 \int_0^{+\infty} \mathrm{e}^{-(t-t')/\tau_p^2 - t'/\tau_c}\, dt'$,
I_2 is second term, $I_2 = -\mu_e E_{DC} I_{opt}^0 \int_0^{+\infty} \mathrm{e}^{-(t-t')/\tau_p^2 - t'/\tau_c}\, e^{-t'/\tau_s} dt'$.
The expression under the integral sign is product of three exponents and subjected to a transformation in order to obtain the result of integration.
The transformation includes such steps as variable and the lower limit of integration changing.

Let's consider integral first term in (2)

$$\int_0^{\infty} \mathrm{e}^{-(t-t')/\tau_p^2 - t'/\tau_c}\, dt' = I_1 \tag{3}$$

Let's in expression (3) denote

$$x = \frac{1}{\tau_p}, \quad y = \frac{1}{\tau_c} \quad , \tag{4}$$

And get such expression

$$\int_0^{\infty} \exp\left(-(t-t')^2 x^2 - t'y\right) dt' = I_1, \tag{5}$$

by definition of complimentary error function

$$erfc(\varsigma) = \frac{2}{\sqrt{\pi}} \int_{\varsigma}^{\infty} e^{-b^2}\, db\,, \tag{6}$$

As it is known [2, p.322] there is substitution for variable changing

$$t \cdot x + \frac{y}{2x} = b, \tag{7}$$

After differentiation (7)

$$db = dt\,, \tag{8}$$

We get after substitution (7), (8) into (6)

$$\int_0^\infty \exp\left(-tx + \frac{y}{2x}\right)^2 dt = \frac{1}{x} erfc\left(tx + \frac{y}{2x}\right)\frac{\sqrt{\pi}}{2}, \tag{9}$$

From expression (7) squaring

$$b^2 = \left(tx + \frac{y}{2x}\right)^2 = t^2x^2 + 2tx\frac{y}{2x} + \frac{y^2}{4x^2} = t^2x^2 + ty + \frac{y^2}{4x^2}, \tag{10}$$

After transfer of terms

$$t^2x^2 + ty = -b^2 + \frac{y^2}{4x^2}\,, \tag{11}$$

$$\int_0^\infty \exp\left(-t^2x^2 - ty\right)dt = \int_0^\infty \exp\left(-b^2 + \frac{y^2}{4x^2}\right)dt = \frac{\exp\left(\frac{y^2}{4x^2}\right)}{x} erfc\left(\frac{y}{2x} + xt\right)\frac{\sqrt{\pi}}{2}, \tag{12}$$

Expression (12) differs from expression (9) by multiplicand $\exp\left(\frac{y^2}{4x^2}\right)$.

Finally add and subtract t / τ_c and group second and third term and change terms order in first bracket they in second degree

$$\begin{aligned} &-\left(t - t'\right)^2 x^2 - t'y = -\left(t - t'\right)^2 x^2 - t'y + ty - ty = \\ &= -\left(t - t'\right)^2 x^2 - \left(t - t'\right) y - ty \end{aligned} \tag{13}$$

Denote $a = ty$

$$-\left(t - t'\right)^2 x^2 - t'y = -\left(t - t'\right)^2 x^2 - (t - t')y - a\,, \tag{14}$$

Consider auxiliary expression

$$-t^2x^2 - ty + a\,, \tag{15}$$

Substitute (14) in integral gives

$$\int_0^\infty \exp(-t^2x^2 - ty + a)dt = \frac{\sqrt{\pi}\cdot\exp\left(a + \frac{y^2}{4x^2}\right)erfc\left(xt + \frac{y}{2x}\right)}{2x}, \tag{16}$$

In expression (16) as compare to (12) appears second summand in exponent argument

As to second integral I_2 by analogue with exception

$$y = \frac{1}{\tau_{cs}},\ \frac{1}{\tau_{cs}} = \frac{1}{\tau_c} + \frac{1}{\tau_s}, \tag{17}$$

From back substitution of expression (4) into expression (15) we get expression what we sought

$$J(t) = \tau_p \frac{\sqrt{\pi}}{2}\mu_e E_{DC} I_{opt}^0 \left\{\exp\left(\frac{\tau_p^2}{4\tau_c^2} - \frac{t}{\tau_c}\right)erfc\left(\frac{\tau_p}{2\tau_c} - \frac{t}{\tau_p}\right) - \exp\left(\frac{\tau_p^2}{4\tau_{cs}^2} - \frac{t}{\tau_{cs}}\right)erfc\left(\frac{\tau_p}{2\tau_{cs}} - \frac{t}{\tau_p}\right)\right\} \tag{18}$$

To verify expression (18) derived analytically was used software Maple and result from Maple is coincided with expression (18) so proof result rightness.

And now compare expression with known expression [1-3].
An approximation of the physics of these emitters, where the generated photo-current an incident optical, femtosecond pulse is given by [1, p.64]

$$I(t) = \frac{\sqrt{\pi}}{2}\mu_e E_{DC} I_{opt}^0 \left\{\exp\left(\frac{\tau_p^2}{4\tau_c^2} - \frac{t}{\tau_c}\right)erfc\left(\frac{\tau_p}{2\tau_c} - \frac{t}{\tau_p}\right) - \exp\left(\frac{\tau_p^2}{4\tau_{cs}^2} - \frac{t}{\tau_{cs}}\right)erfc\left(\frac{\tau_p}{2\tau_{cs}} - \frac{t}{\tau_p}\right)\right\} \tag{19}$$

Expression (18) differs from expression (19) by multiplicand $\frac{1}{x} = \tau_p$.

Only in expression (15) we consider auxiliary expression $-t^2x^2 - ty + a$ instead of $-(t-t')^2 x^2 - (t-t')y - a$.

Let's use Maple and get correct solution. It is after substitution (4)

$$I_1 = -\frac{\sqrt{\pi}}{2}\mu_e E_{DC} I_{opt}^0 \frac{\sqrt{\pi}\exp\left(-x^2t^2 + \frac{(4tx^2 - y)^2}{4x^2}\right) erf\left(-xt' + \frac{2tx^2 - y}{2x}\right)}{2x} =$$

$$= \frac{1}{2}\tau_p \frac{\sqrt{\pi}}{2}\mu_e E_{DC} I_{opt}^0 \sqrt{\pi}\exp\left(-\frac{t^2}{\tau_p^2} + \frac{\left(\frac{4t}{\tau_p^2} - \frac{1}{\tau_c}\right)^2}{4\frac{1}{\tau_p^2}}\right) erf\left(-\frac{t'}{\tau_p} + \frac{\frac{2t}{\tau_p^2} - \frac{1}{\tau_c}}{2\frac{1}{\tau_p^2}}\right) =$$

(20)

$$= \frac{1}{2}\tau_p \frac{\sqrt{\pi}}{2}\mu_e E_{DC} I_{opt}^0 \sqrt{\pi}\exp\left(-\frac{t^2}{\tau_p^2} + \frac{4t}{\tau_p^2} - \frac{2}{\tau_c} + \left(\frac{\tau_p}{\tau_c}\right)^2 \frac{1}{4t}\right) erf\left(-\frac{t'}{\tau_p} + t - \frac{\tau_p^2}{2\tau_c}\right).$$

The problem of each research is in contradiction. This research results have its own contradiction between known formula (19) and derived by us formula (18). The two formula differ by multiplicand τ_p. Next step was to check by means automated calculation with Mapple software to be sure that our result without error. And our results was confirmed with the aid of Maple software.

3. CONCLUSION

The subject of this report is a derivation of expression for photocurrent density in terahertz spectroscopy. The mathematical model of the photocurrent is a convolution of the laser radiation pulse irradiating the surface of the material under test and the current density, which in turn is the product of the carrier concentration, charge, and velocity. The result of calculation partially coincide with known result but could be improved if instead of taking tabular integral pay attention to the conditions of a particular task. There was revised expression for photocurrent density and was received more correct result due to using of Maple.

The issue in every research lies in contradictions. This study's findings exhibit a contradiction between the established formula (19) and the formula we derived (18). The discrepancy between the two lies in the multiplicand. To ensure the accuracy of our results, the subsequent step involved verifying them through automated calculations using Maple software. The confirmation of our results came through the validation process with Maple software, reassuring the absence of errors.

CONFLICT OF INTEREST

The authors stated that there are no conflicts of interest regarding the publication of this article.

AUTHORSHIP CONTRIBUTIONS

Iurii Khoroshailo: Supervision. Nataliia Zaichenko: Experimental and numerical modeling, Methodology, Visualization, Writing – original draft, Olga Zaichenko: Writing – review & editing.

REFERENCES

[1] Lee YS. Principles of terahertz science and technology. Springer Science & Business Media, 2009, 337.

[2] Klokkou N, Gorecki J, Wilkinson JS, Apostolopoulos V. Artificial neural networks for material parameter extraction in terahertz time-domain spectroscopy Optics Express 2022; 30(9): 15583-15595.

[3] Duvillaret L, Gare F, Roux JF, Coutaz JL. Analytical modeling and optimization of terahertz time-domain spectroscopy experiments, using photoswitches as antennas. IEEE Journal of Selected Topics in Quantum Electronics 2001; 7(4): 615-623.

[4] Gradshtein IS, Ryzhik IM. Tables of integrals, sums, series and products. Fizmatgiz, 1963, 1108.

[5] Arjavalingam G, Theophilou N, Pastol Y, Kopcsay GV, Angelopoulos M. Anisotropic conductivity in stretch-oriented polymers measured with coherent microwave transient spectroscopy. The Journal of chemical physics, 1990, 93(1), 6-9.

[6] Nuss MC, Goossen KW, Gordon JP, Mankiewich PM, O'malley ML, Bhushan M. Terahertz time-domain measurement of the conductivity and superconducting band gap in niobium. Journal of Applied Physics, 1991, 70(4), 2238-2241.

[7] Van Exter M, Grischkowsky DR. Characterization of an optoelectronic terahertz beam system. IEEE Transactions on Microwave Theory and Techniques, 1990, 38(11), 1684-1691.

[8] Withayachumnankul W, Fischer BM, Lin H, Abbott D. Uncertainty in terahertz time-domain spectroscopy measurement. JOSA B, 2008, 25(6), 1059-1072.

[9] Jepsen PU, Jacobsen RH, Keiding SR. Generation and detection of terahertz pulses from biased semiconductor antennas. JOSA B, 1996, 13(11), 2424-2436.

[10] Piao ZS, Tani M, Sakai K. Carrier dynamics and THz radiation in biased semiconductor structures. In Terahertz Spectroscopy and Applications, 1999, 3617, 49-56.

[11] Raj A. Quantitative analysis of optical parameters using THz-TDS. Master Thesis Report, University Jean Monnet, 2023, 47.

[12] Li E, Yang J, Zhang K, Li H, Xu Y, Su F, Fang G. (2023). Systematic Study of Two-color Air Plasma Broadband THz-TDS. IEEE Transactions on Terahertz Science and Technology, 2023, 13(5), 476-484.

[13] Cherniak V, Kubiczek T, Kolpatzeck K, Balzer JC. Laser diode based THz-TDS system with 133 dB peak signal-to-noise ratio at 100 GHz. Scientific Reports, 2023, 13(1), 13476.