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Advances in THz Spectroscopy: A Systematic Review of Material Characterization Applications

Erick Reyes Vera[1,], Jorge Montoya-Cardona[1], Vanessa García Pineda[1], Alejandro Valencia-Arias[2], Nelson Gomez-Cardona[1], Francisco Lopez-Giraldo[1], Esteban Gonzalez-Valencia[1]*

[1]Instituto Tecnológico Metropolitano, Medellín, Colombia

[2]Universidad de Los Lagos, Osorno, Chile

[*]Correspondence: E-mail: erickreyes@itm.edu.co

ABSTRACT

Terahertz Time-Domain Spectroscopy (THz-TDS) has emerged as a powerful non-contact, non-destructive tool for probing the dielectric and structural properties of various materials. This systematic review aims to synthesize the latest developments and applications of THz-TDS in material characterization. Following the PRISMA methodology, peer-reviewed articles were selected from the Scopus and Web of Science databases based on strict inclusion criteria. The review identifies three dominant research trends: (i) advances in physical modeling (Debye-Lorentz and Drude-Smith models) for extracting optical parameters, (ii) integration of machine learning techniques for classification and predictive analysis, and (iii) enhancement of system bandwidth and sensitivity through photonic and detector innovations. Findings suggest that while THz-TDS offers high potential across fields such as semiconductors, thin films, and biomaterials, standardization in instrumentation and data analysis remains limited. This paper contributes a research roadmap for more robust THz-TDS applications in quality control, diagnostics, and smart material development.

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1. INTRODUCTION

Terahertz time-domain spectroscopy (THz-TDS) leverages electromagnetic waves in the 0.1–10 THz range, bridging the microwave and far-infrared regions [1, 2]. Over the last decade, the terahertz spectral region has become a highly active area of research not only in spectroscopic analysis but also in the development of high-performance sources, detectors, and waveguides, enabling more durable, efficient, and accessible THz platforms for scientific and industrial applications [1, 3-9].

One of the principal benefits of THz-TDS is its ability to probe dielectric, structural, and spectroscopic characteristics of materials in a non-contact, non-destructive manner [6, 9, 10]. Unlike many other spectroscopic methods, THz radiation is highly transparent in numerous dielectric media (such as polymers and biological tissues) while interacting preferentially with polar compounds, making it an excellent tool for detecting chemical species and structural fingerprints [6, 9, 10]. In materials science, THz spectroscopy enables broadband measurement of complex permittivity and refractive index, which is useful for studying semiconductors, polymers, multilayer composites, and biomolecules. Moreover, the intrinsically low photon energy of THz radiation reduces sample damage and prevents ionization, making it suitable for life sciences, pharmaceuticals, and soft-matter applications [11].

These characteristics have driven widespread use across multiple sectors. In semiconductors, THz-TDS supports nondestructive examination of microelectronic devices and identification of material defects; in biological contexts, it enables tissue categorization, biomolecular fingerprinting, and cancer diagnosis [5]. THz spectroscopy has also proven useful for detecting explosives and controlled substances. Furthermore, its integration with machine learning has gained traction for processing complex spectral data in industrial settings, including the detection of bisphenols in chemical mixtures.

Despite its promise, broader adoption of THz-TDS is constrained by fragmented domain knowledge, the absence of standardized protocols, and relatively high implementation costs, which hinder integration into conventional analytical workflows. Practical limitations in spectral resolution, sensitivity, and environmental robustness further restrict deployment beyond specialized facilities [12]. Addressing these challenges will require consolidating current findings, standardizing methodologies, and promoting interoperability across application domains. Recent advances in THz technology, signal modeling, and artificial intelligence offer pathways to more precise parameter extraction, improved repeatability, and greater accessibility.

In this context, the objective of this review is to evaluate the potential of terahertz spectroscopy for material characterization by analyzing its applications, advantages, and limitations relative to conventional techniques. To guide this investigation, we pose the following research questions:

(i) What structural, electrical, and spectral properties of materials can be characterized using terahertz spectroscopy?

(ii) What are the main applications of terahertz spectroscopy in material characterization?

(iii) What advantages does terahertz spectroscopy offer compared to other techniques?

(iv) What technical and economic limitations hinder the implementation of terahertz spectroscopy in industrial and scientific environments?

(v) How are machine-learning algorithms being applied in terahertz-range material characterization?

(vi) What recent advances have improved the performance of terahertz spectroscopy for material analysis?

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(vii) How can the use of terahertz spectroscopy in material characterization be optimized?

To answer these questions, this article adopts a structured approach to consolidating existing knowledge on terahertz spectroscopy for material analysis. Using a systematic review methodology, we organize dispersed findings from multiple disciplines, identify methodological gaps, and propose future research directions. The discussion highlights emerging trends, challenges, and technical strategies to enhance sensitivity, resolution, and accessibility across scientific and industrial domains. The article is organized into introduction, methodology, results, discussion, and conclusions to ensure a comprehensive and rigorous analysis.

2. METHODS

This review strictly follows the PRISMA 2020 (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) guidelines to ensure a rigorous, transparent, and reproducible approach to identifying, selecting, and analyzing the scientific literature on terahertz spectroscopy applied to material characterization [13]. We registered our protocol a priori and used the PRISMA 2020 checklist to guide each phase—identification, screening, eligibility, and inclusion—thereby minimizing bias and enhancing traceability. A PRISMA flowchart (**Figure 1**) illustrates the number of records identified, reviewed, excluded, and included, ensuring that the selection process remains fully transparent.

2.1. Methods Eligibility Criteria

We established strict inclusion and exclusion criteria to ensure that only high-quality, directly relevant studies using THz-TDS for material characterization were considered. Eligible studies were original, peer-reviewed research articles published in indexed journals, written in English, and focused on the application of THz-TDS (generally within the 0.1–10 THz range) to extract optical or dielectric properties (such as refractive index, absorption coefficient, or complex permittivity) or to determine structural features of solids, liquids, or composite systems. We excluded review articles, conference proceedings, theses, book chapters, and publications that lacked full-text access or had metadata inconsistencies.

The screening process was conducted in three phases. In the first phase, we removed duplicate records and entries with indexing errors or insufficient information in the title or abstract. The second phase excluded articles without full-text access, as their content could not be evaluated using standard academic criteria. In the final phase, we conducted critical full-text readings.

Studies were excluded if they mentioned terahertz spectroscopy but did not apply it within a material characterization framework or focused on unrelated technical or conceptual issues. This final step ensured that only studies with a clear and coherent alignment to the review's objectives were retained.

2.2. Information Sources

We conducted our systematic literature search using Scopus and Web of Science (WoS), two of the most comprehensive peer-reviewed databases for applied physics, materials engineering, and spectroscopic technologies. Scopus (Elsevier) indexes journals, conference proceedings, and books from as early as 1960 and offers advanced bibliometric tools such as citation tracking and h-index metrics.

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Web of Science (Clarivate) provides an even broader historical scope, indexing literature from as early as 1900, with standardized metadata fields, strict editorial curation, and integrated citation analytics that support thematic clustering and longitudinal trend analysis.

By using both platforms, we mitigated regional and publisher-related biases and assembled a dataset representative of global research activity in terahertz spectroscopy. Combined searches across Scopus and WoS have been shown to capture over 95% of high-impact journals in the physical sciences [14]. To address minor geographic and institutional gaps, we also manually searched the reference lists of key articles.

2.3. Search Strategy

Based on our predefined eligibility criteria, we developed tailored search queries for each database to retrieve original research articles on THz-TDS for material characterization. In Scopus, the search string was: TITLE (spectrosco* AND terahertz AND characterization). For Web of Science, the search query used was: TS = (spectrosco* AND terahertz AND characterization), where "TS" refers to a topic search that includes titles, abstracts, and keywords. Both searches were limited to English-language articles and filtered by the document type "Article."

Searches were performed in April 2025 and covered all available publication years. The results (including abstracts, keywords, and citation data) were exported into a reference management tool to eliminate duplicates. We also manually screened the bibliographies of highly cited studies and recent review articles to retrieve additional relevant works that were not captured through the primary database searches. This systematic strategy ensured that the final corpus reflects the most recent, relevant, and methodologically robust research on terahertz spectroscopy in material characterization.

2.4. Study Selection

The study selection was conducted in three sequential phases. The first phase involved screening article titles to eliminate studies unrelated to terahertz spectroscopy or material characterization. In the second phase, abstracts were reviewed to ensure thematic and methodological alignment with the objectives of the review. The final phase consisted of full-text assessments to evaluate each article's relevance, analytical rigor, and contribution to the field. This structured, multi-step approach ensured that the initial pool of records was refined systematically, improved the consistency and reliability of the final dataset, and resulted in the inclusion of only those studies that met high scientific standards and were directly aligned with the review scope.

2.5. Data Processing

Data processing was conducted using Microsoft Excel due to its versatility in organizing, filtering, and analyzing bibliographic datasets. Exported records were compiled into structured spreadsheets, where key variables (such as authorship, publication year, country of origin, journal source, keywords, and study objectives) were systematically coded. This structured approach enabled efficient identification of thematic patterns, removal of duplicates, and verification of inclusion criteria for each entry.

In addition, Excel was used to generate frequency tables and visual summaries to support preliminary quantitative analyses. Centralizing all procedures within a reproducible data management framework ensured transparency, traceability, and consistency across the review process.

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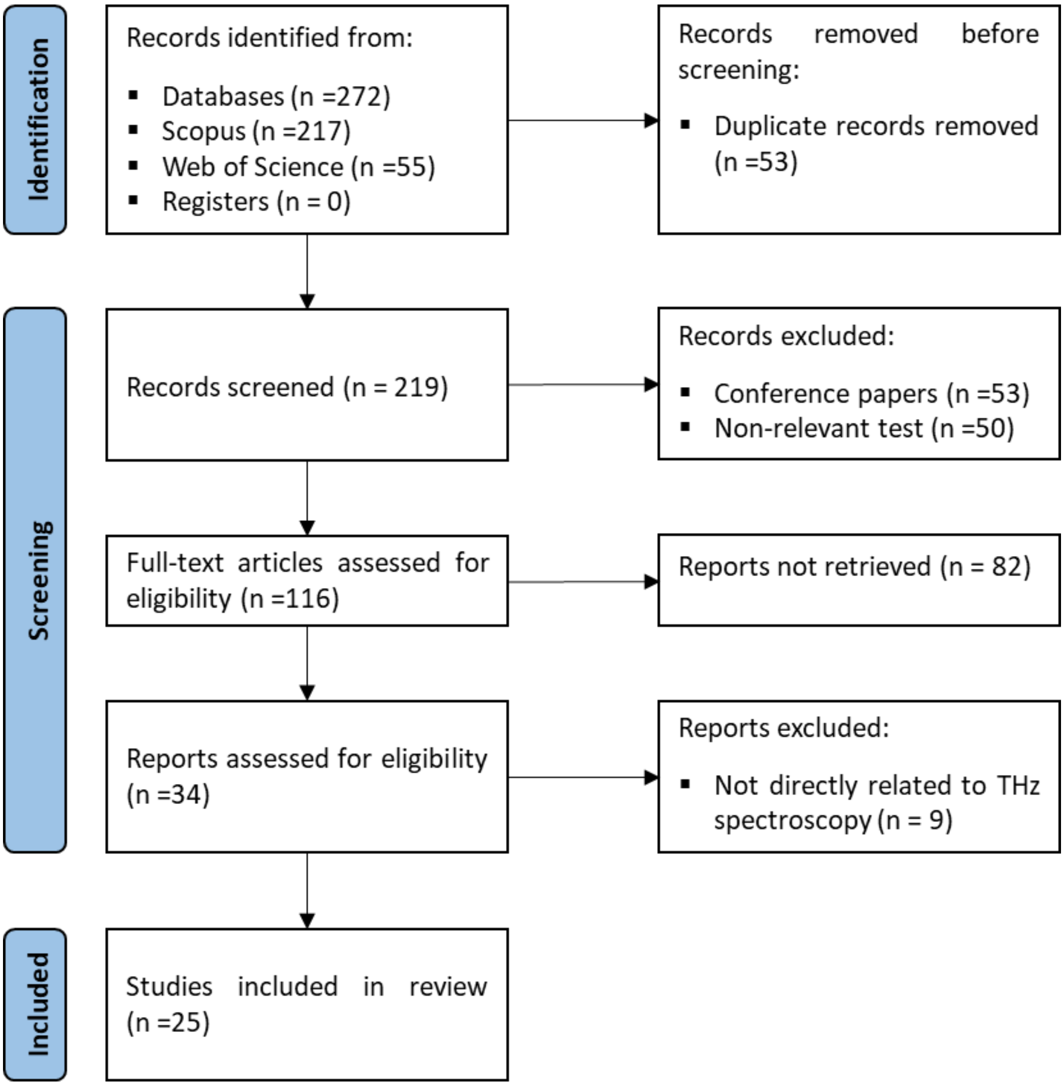

Figure 1. PRISMA 2020 flow diagram outlining the study selection process based on searches in Scopus and Web of Science. Created by the authors.

2.6. Risk of Bias

Potential sources of bias were critically assessed throughout the review process. First, selection bias may have been introduced by limiting the search to Scopus and Web of Science, potentially excluding relevant studies not indexed in these databases. Second, thematic bias may have resulted from the formulation of search queries, which could inadvertently narrow the scope of retrieved literature. Third, reporting bias was considered, recognizing the common tendency in academic publishing to emphasize studies with significant or visually compelling outcomes.

To mitigate these risks, all screening decisions were subjected to peer review, and the inclusion criteria were independently cross-validated by multiple researchers. This collaborative and transparent approach minimized subjectivity and enhanced the overall methodological rigor and credibility of the review.

3. RESULTS AND DISCUSSION

The results of this review are organized according to the core research questions to provide a clear and structured overview of how THz-TDS has been applied to material

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characterization. This structure enables a detailed examination of technical implementations, analytical methodologies, and application-specific outcomes. Key trends, current limitations, and opportunities for methodological improvement are highlighted across a wide range of material types. **Table 1** presents a concise summary of the twenty-two studies included in the review, detailing the THz-TDS modality, application domain, and the principal variables measured. Transmission-mode THz-TDS emerges as the most widely used configuration, appearing in over two-thirds of the reviewed studies. The remaining studies employ alternative setups, including attenuated total reflection (ATR), polarimetric systems, continuous-wave sources, and reflection-mode geometries, each selected to address specific experimental challenges. Across the reviewed literature, the most frequently extracted parameters are the refractive index, absorption coefficient, and phase delay. More advanced analyses focus on the retrieval of complex permittivity spectra, quantification of dielectric contrast, and identification of vibrational modes associated with molecular structures. Furthermore, several studies incorporate multivariate classification techniques, such as principal component analysis (PCA) and support vector machines (SVM), to resolve complex material signatures and enhance interpretability.

Table 1. Characteristics of included studies: THz-TDS configuration, application domain, key parameters measured, and reference.

Title	THz-TDS Modality	Application Domain	Variables Studied	Reference
Characterization of Oils and Oil Mixtures using Terahertz Time-Domain Spectroscopy	Transmission	Edible and industrial oils and their blends	Refractive index; absorption coefficient; phase difference	[15]
Experimental characterization of a fully polarimetric pulsed terahertz spectroscopy system	Polarimetric (quartz wedge)	Birefringent quartz crystal	Electric-field vector components; phase retardation; polarization state	
Pigments, minerals, and copper-corrosion products: THz-CW spectroscopic characterization of antlerite and atacamite	Continuous-wave	Cultural-heritage pigments	Absorption coefficient; spectral selectivity; relative concentration in mixtures	[16]
Terahertz Spectroscopic Characterization for Carbon-based Materials	Transmission	Graphite; carbon nanotubes; nanofibers	Absorption bands; electronic properties; structural differences	
Terahertz Spectroscopy for the Characterization of Excised Human Breast Tissue	Transmission (TPS Spectra 3000)	Ex vivo human breast tissue (healthy vs. cancerous)	Complex dielectric constant; water-content absorption; sample-holder materials	[17]
Analysis and characterization of 5-fluorouracil based on terahertz spectroscopy	Transmission with concentration series	Pharmaceutical APIs (5-fluorouracil)	Refractive index; absorption coefficient; concentration correlation	

Table 1 (Continue). Characteristics of included studies: THz-TDS configuration, application domain, key parameters measured, and reference.

Title	THz-TDS Modality	Application Domain	Variables Studied	Reference

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Broadband terahertz spectroscopy and its application to the characterization of thin films	Ultrafast pulses (15 fs & 5 fs) in reflection geometry	Dielectric thin films; pump-probe measurements	Complex permittivity; phase dispersion	[18]
A review: Terahertz spectroscopy as a viable dynamic tool for protein and organic molecules characterization	Review (primarily THz-TDS)	Proteins; organic macromolecules	Vibrational modes; resonance absorption; protein structural dynamics	
Characterization and Classification of Coals and Rocks Using THz-TDS + PCA/SVM	Transmission + PCA & SVM	Unmanned mining: coal–rock interface recognition	Absorption coefficient; refractive index; dielectric constant; moisture; ash/volatile content	[19]
Characterization and evaluation of oil shale based on terahertz spectroscopy: A review	Review of multiple THz methods	Oil shale	Anisotropy; kerogen content; absorption peaks; organic distribution	
Characterization of field-effect terahertz detectors using THz-TDS with antenna-coupled FETs	Transmission (FET–antenna configuration)	AlGaN/GaN FET-based THz detectors	Transmission coefficient; spectral response; detector sensitivity	[20]
Characterization of LPCMO thin films by THz-TDS + Drude–Smith modeling	Transmission + Drude–Smith fit	$La_{0.33}Pr_{0.34}Ca_{0.33}MnO_3$ (LPCMO) thin films	Optical conductivity; scattering time; carrier density; non-Drude response	
Characterization of materials and other applications of terahertz spectroscopy in the time domain	Transmission	Emerging applications: THz imaging; sensors; devices	Dielectric properties; optical constants; spectral response across GHz–THz	[21]
Characterization of Ultrathin Conductive Films by THz-TDSE	Time-domain spectroscopic ellipsometry with ultrathin-film model	Rare-earth nickel oxide films	Surface conductivity; dielectric constant; temperature dependence; polarization distortion	[22]
Characterization of wheat varieties using THz-TDS + PLS/iPLS	Transmission + PLS/iPLS (0.2–2.0 THz)	Rapid, nondestructive wheat variety discrimination	Absorption spectra; refractive index; moisture; protein; gluten content	
Dendrimer-based THz-TDS and applications in molecular characterization	Electro-optic sampling + DFG	Explosives; macromolecules	Molecular vibrational modes; absorption spectra; molecular-dynamics simulations	[23]

Table 1 (Continue). Characteristics of included studies: THz-TDS configuration, application domain, key parameters measured, and reference.

Title	THz-TDS Modality	Application Domain	Variables Studied	Ref.

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Dielectric characterization of $[Fe(NH_2\text{-}trz)_3]Br_2\cdot H_2O$ spincrossover compound	Transmission	Iron spin-crossover complex	Complex refractive index; transfer function; temperature dependence	
Phase-change material films: fabrication & characterization by THz-TDS + DSC, TGA, SEM	Transmission + thermal & microscopic techniques	Photocrosslinked phase-change materials	Refractive index; THz absorption; thermal properties; FTIR spectra	[24]
Improved sample characterization in THz reflection imaging and spectroscopy	Reflection + baseline simulation	Liquids (e.g., isopropanol)	Refractive index; absorption coefficient; phase; baseline correction	
THz reflection-mode characterization of graphene conductivity on metal-backed dielectrics + Drude–Smith post-processing	Reflection (oblique incidence) + generalized Drude–Smith	Graphene on metal-backed substrates	Graphene conductivity; substrate thickness; dielectric dispersion; amplitude spectra	[27]
THz spectroscopic characterization & DFT of carbamazepine cocrystals with nicotinamide, saccharin & fumaric acid	Transmission + DFT-phonon calculations (VASP, Phonopy)	Pharmaceutical cocrystals of carbamazepine	Helmholtz free energy; vibrational modes; unit-cell energy; vibrational contributions to stability; hydrogen bonds	
Terahertz/far-IR characterization of Laggera decurrens essential oil	FT-IR + DFT calculations	Essential oils (timol; carvacrol; timoquinone)	Absorption spectra; vibrational modes	[28]

As shown in **Figure 2**, the primary application areas where THz-TDS has demonstrated the greatest impact are semiconductor structures, optical substrates, and polymeric films. Collectively, these three categories account for half of the studies reviewed. This distribution reflects the well-established capability of THz-TDS to probe charge carrier dynamics and dielectric properties in semiconductors, as well as its effectiveness as a non-destructive method for analyzing thin dielectric layers at the nanometer scale.

Beyond these dominant domains, THz-TDS has also proven valuable in several other scientific and industrial contexts. These include the quantitative analysis of active pharmaceutical ingredients in complex formulations, the detection of plastic explosives for security applications, the characterization of printed electronics, and the study of chalcogenide glasses for photonic systems. In addition, **Figure 2** highlights several emerging and less frequently explored areas, such as antibody complexes, metallic alloys, ceramic coatings, mineral inclusions, adhesive interfaces, bone structures, and painted surfaces. In these cases, the high penetration depth and sensitivity of THz-TDS to compositional variations make it a powerful tool for characterizing heterogeneous materials with complex internal architectures. As illustrated in **Figure 3**, all reviewed studies emphasize the non-destructive nature of THz-TDS, a critical feature that enables probing of materials without compromising sample integrity. Contactless measurement, another frequently reported advantage, is particularly beneficial when analyzing delicate or biological specimens [29, 30]. High precision in refractive index determination is also consistently noted, underscoring the technique's reliability for accurate dielectric profiling.

Beyond these core capabilities, **Figure 3** also reveals frequent emphasis on high spectral resolution, electrical property mapping, repeatability, hydrogen bond sensitivity, and soft

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biomolecule detection. High spectral resolution enables researchers to resolve closely spaced vibrational features, while dielectric mapping provides spatial insight into local variations in conductivity or permittivity. The sensitivity of THz-TDS to hydrogen bonding offers valuable insights for studies involving aqueous solutions and biomolecular interactions. Moreover, THz-TDS's responsiveness to low-energy vibrational modes enhances its utility in characterizing soft matter, including polymers and protein-based materials. However, none of the reviewed studies reported uncertainty estimates or validated their findings using complementary spectroscopic techniques such as Fourier Transform Infrared Spectroscopy (FTIR) or Nuclear Magnetic Resonance (NMR).

This omission limits cross-laboratory comparability of refractive index values, conductivity profiles, and spectral fingerprints. To improve reproducibility and scientific robustness, future THz-TDS studies should incorporate uncertainty ranges or confidence intervals for key extracted parameters. Validation against benchmarked techniques, inclusion of replicate datasets, clear bandwidth specifications, and inter-laboratory calibration protocols would significantly enhance the reliability and comparative utility of THz measurements.

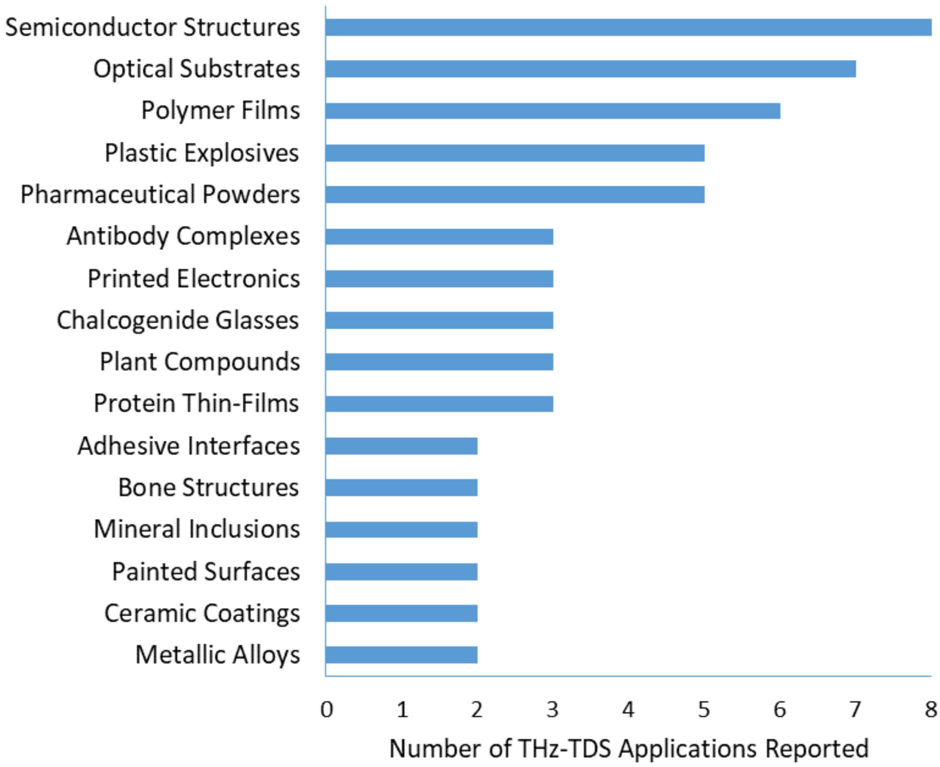

Figure 2. Distribution of THz-TDS applications by material type based on the systematic review of twenty-two selected studies. compiled by the authors from Scopus and Web of science.

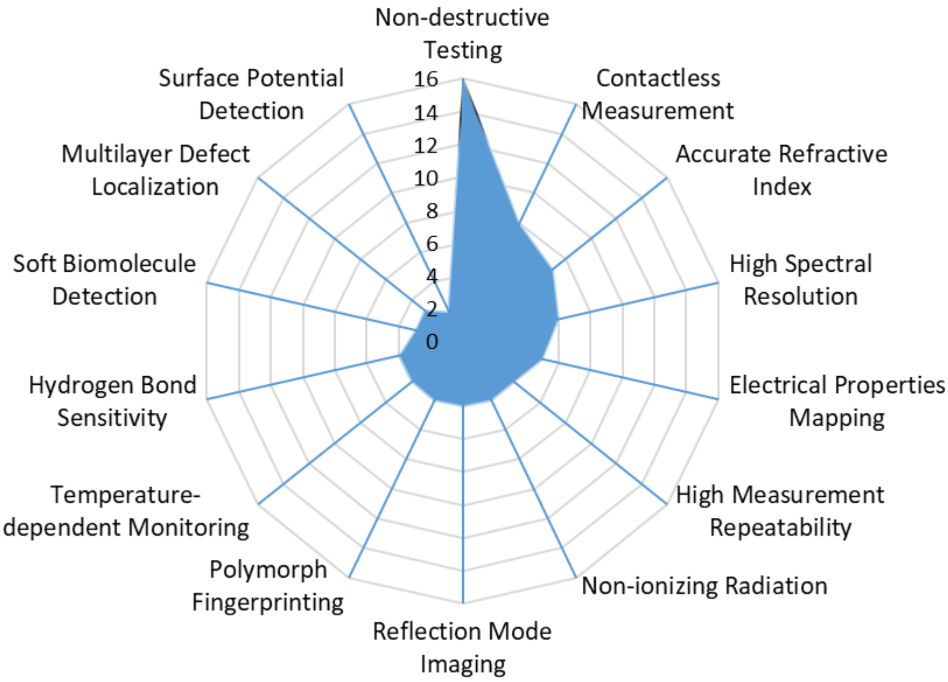

Figure 3. Number of THz-TDS studies reporting specific metrological or functional attributes, including non-destructiveness, spectral resolution, and contactless operation. Data compiled by the authors from Scopus and Web of Science.

Figure 4 summarizes the most frequently reported technical limitations and practical challenges associated with THz-TDS. The most prevalent constraints are material-specific, including sample thickness variation, structural heterogeneity, and trace-level impurities, all of which can reduce spectral quality [31, 32]. In addition, many studies note the requirement for nitrogen-purged enclosures to mitigate atmospheric water vapor absorption, a known source of signal distortion in the THz range.

Other commonly cited limitations include high equipment acquisition and maintenance costs, the need for specialized components, and the computational complexity of THz data modeling. Sample preparation is often labor-intensive, particularly for multilayer structures or highly absorbing materials. Less frequently reported, but still significant, obstacles include signal attenuation, sensitivity to optical misalignment, and difficulties in detecting polymorphic phase transitions.

Overall, **Figure 4** underscores that while THz-TDS provides a rich set of material insights, its practical deployment requires meticulous control over sample configuration, environmental conditions, and instrumentation parameters.

Figure 5 depicts recent advancements that researchers have implemented to enhance the sensitivity and resolution of THz-TDS. Among these, the ongoing development of physical and mathematical modeling has significantly improved the accuracy of parameter extraction and reduced interpretive ambiguity. Phase-sensitive imaging techniques are gaining prominence for their ability to enhance contrast in heterogeneous materials, while optimized attenuated total reflection (ATR) configurations have enabled more consistent detection of hydration states.

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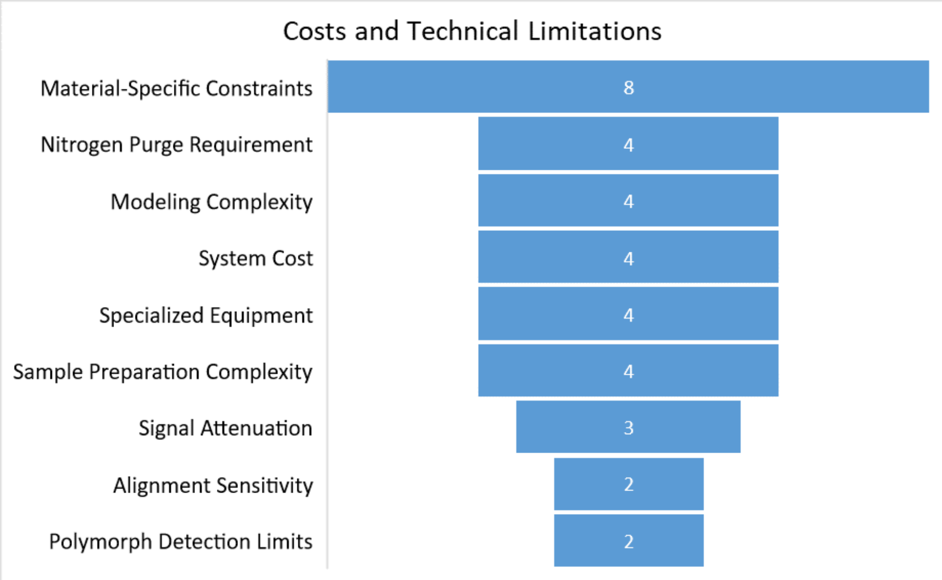

Figure 4. Most reported costs and technical limitations. Own elaboration based on Scopus and Web of Science.

In parallel, temperature-correlated investigations have provided deeper insight into how thermal dynamics affect the terahertz response, with several studies reporting sub-picosecond temporal resolution in refractive index mapping. Additionally, modern data processing strategies (such as spectral denoising and machine learning–based pattern recognition) have proven effective in distinguishing closely related polymorphic forms. Taken together, these developments reflect a rapidly evolving analytical technique capable of delivering increasingly precise and high-resolution material characterizations.

As shown in **Figure 6**, THz-TDS is most frequently applied in three key areas of biomaterial optimization: integration with biocompatible matrices, longitudinal monitoring of polymer degradation, and label-free biosensing applications. Other high-frequency themes include protein detection and tissue differentiation, where the technique's sensitivity to molecular vibrational modes allows for fine discrimination of biomolecular structures [26]. Additional applications (such as polymorph control, non-destructive diagnostics, and biofilm characterization) further demonstrate the versatility of THz-TDS in probing structural and chemical heterogeneity within soft biological systems, without compromising sample integrity.

Beyond these central domains, several studies also explore niche or emerging applications, including food quality assessment, optimization of chalcogenide glass–based biomaterials, evaluation of implant surfaces, hydration-sensitive mapping, and surface interaction analyses.

Organizing the findings around targeted research questions enabled the identification of recurring methodological patterns, technological innovations, and critical limitations. **Figure 6** synthesizes these insights by highlighting both well-established research trajectories and existing gaps, such as the absence of standardized protocols for implant testing and the lack of systematic strategies for long-term biofilm monitoring. Collectively, these findings underscore the expanding role of THz-TDS as a non-invasive, high-resolution analytical platform for advanced biomaterials research in both academic and industrial contexts.

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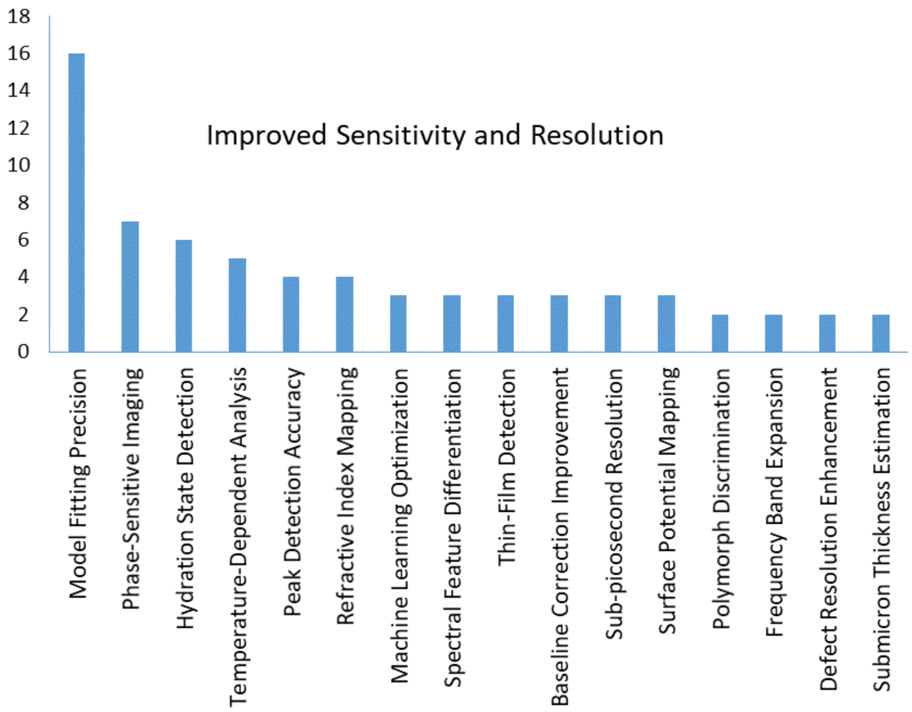

Figure 5. Improvements in sensitivity and resolution. Own elaboration based on Scopus and Web of Science.

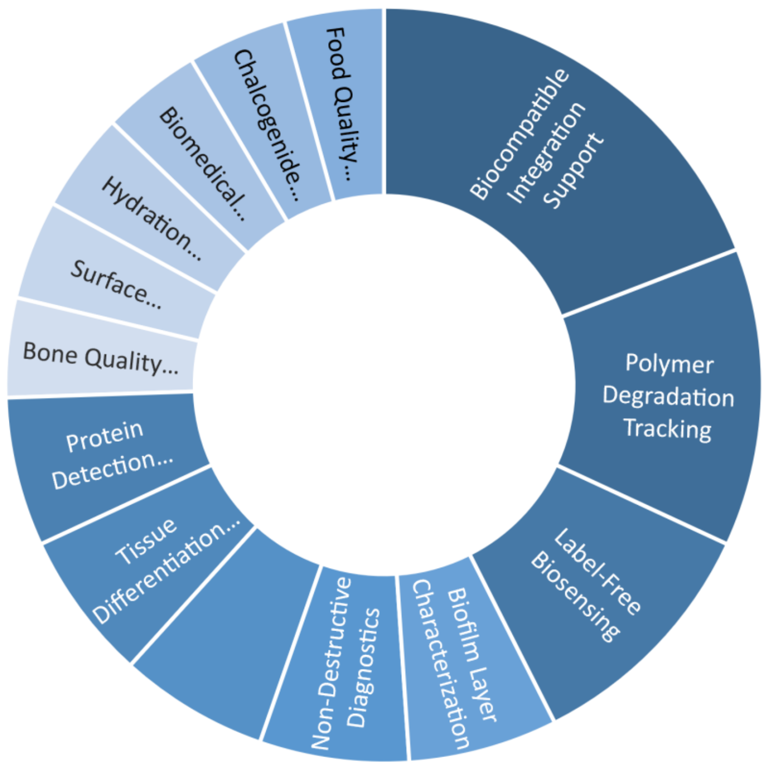

Figure 6. Applications for biomaterials optimization. Own elaboration based on Scopus and Web of Science.

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3.2. Applications of Thz Spectroscopy for Material Characterization

3.2.1. Dielectric characterization of semiconductors and thin films

Dielectric characterization of semiconductors and thin films using THz-TDS has evolved substantially in response to the semiconductor industry's demand for rapid, non-contact metrology across increasingly thin and complex material systems. Initially limited to basic amplitude and phase measurements in transmission mode, the field has advanced toward full ellipsometric extraction in reflection mode, enabling characterization across a broader range of film thicknesses, absorptive properties, and substrate types.

A significant leap beyond bulk measurements came with the introduction of differential time-domain spectroscopy (DTDS), which subtracts a reference waveform from the sample response and compares the amplitude ratio. This technique lowered the minimum measurable thickness into the submicron range at frequencies below 10 GHz, representing an order-of-magnitude improvement over conventional THz-TDS for ultrathin coatings [33].

Building upon this enhanced sensitivity, researchers extended visible-light ellipsometry into the THz domain using goniometric THz spectroscopy (GTDS). By mounting an ultrafast emitter and detector on a θ–2θ gonioscope and scanning reflectance near Brewster's angle, they fitted phase jumps to Fresnel equations and extracted dielectric constants from micrometer-thick FLARE, TiO_x, and PZT films [34].

As demand shifted toward opaque and conductive coatings, reflection-mode THz-TDS methods became indispensable. One implementation captured both amplitude ratios and phase shifts between p- and s-polarizations in a reflection geometry, recovering the complex permittivity of doped GaAs films, matching Drude model predictions, and resolving soft-phonon dispersion in ultrathin $SrTiO_3$ layers on opaque substrates [35].

Further advances targeted heterostructures and band alignment in semiconductor materials. One study introduced terahertz excitation spectroscopy to measure conduction-band offsets in GaAsBi-GaAs junctions (Karpus et al., 2018). Another examined analytical models for THz photoconductivity in highly doped films and showed that common Drude approximations underestimated carrier mobility by more than 50% in perovskite iodide layers, proposing corrected formulas valid for dark conductivities up to $10^4\ \Omega^{-1}\cdot cm^{-1}$ [36].

Expanding on amplitude-only reflection strategies, researchers introduced a Gires–Tournois etalon protocol using three reference spectra (mirror, bare substrate, and sample) to quantify sheet resistance across four decades in transparent conducting oxides, 2D semiconductors, and metals [37]. Shortly afterward, it was demonstrated that combining amplitude-only reflection data with a generalized Drude–Smith model enabled precise, non-destructive conductivity measurements of graphene on metal-backed substrates [38].

From a materials engineering perspective, transmission-mode THz-TDS was used to investigate the effects of rapid thermal annealing on indium tin oxide (ITO) films. By fitting Drude–Smith models to amplitude and phase spectra between 0.2 and 1 THz, the study extracted DC resistivities of 10^{-3}-$10^{-4}\ \Omega\cdot cm$, mobilities up to $47\ cm^2/V\cdot s$, carrier densities around $10^{21}\ cm^{-3}$, and scattering times ranging from 8 to 21 femtoseconds [39].

Finally, two milestone studies in 2024 extended THz-TDS mapping to compound semiconductors. One employed transmission-mode THz-TDS with simplified Drude modeling and Nelder–Mead optimization to non-destructively map carrier concentrations, matching manufacturer specifications over 2–5 hour wafer scans [40].

Another achieved wide-range reflection-mode resistivity mapping of silicon (10^{-3}–$10^2\ \Omega\cdot cm$) using peak-ratio and full-bandwidth optimization fits, successfully imaging radial

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striations with 1 mm lateral resolution, surpassing the spatial precision of traditional four-point probe methods [41].

3.2.2. Structural analysis of pharmaceutical compounds and biomolecules

Terahertz spectroscopy has emerged as a versatile, non-destructive analytical technology with numerous applications in the pharmaceutical and biomedical industries. One of its most significant uses is the characterization of solid-state drugs, as crystalline form directly affects key properties such as solubility and bioavailability. THz spectra are highly sensitive to lattice vibrations and intermolecular interactions, allowing for precise differentiation among polymorphs, co-crystals, and amorphous forms [42]. Early studies used THz-TDS to quantify the crystalline forms of drugs such as theophylline and ranitidine hydrochloride [43, 44]. More recent research has included structural investigations of acyclovir polymorphs [45], monitoring of mechanochemical co-crystal formation [46], and characterization of pyrazinamide, diflunisal, and indomethacin co-crystals [47, 48].

THz spectroscopy has also been instrumental in exploring the microstructure of solid dosage forms. A linear relationship between the effective refractive index and tablet porosity was demonstrated using THz-TDS [49]. Investigations into tablet anisotropy and compressibility further related these structural features to porosity and mechanical strength [50]. Pulsed THz imaging was applied to develop calibration models for chemical constituents in four-component tablets [51]. In more recent applications, THz-TDS has been used to probe porosity in 3D-printed tablets [52] and to non-destructively track particle-size variation in granular compacts [53].

In process analytical technology (PAT), THz-TDS is valued for its ability to monitor critical variables in real time without halting production. Chemometric techniques have been widely integrated with THz spectroscopy for both qualitative and quantitative analysis of medicinal compounds, including complex mixtures [54]. Applications include drug identification and quality control [55], as well as prediction of active-ingredient concentration and tablet density using multivariate analysis [56]. Several systematic reviews have emphasized the growing role of real-time, non-destructive THz methods in PAT monitoring and control [57, 47].

In the biomedical domain, THz-TDS has been widely studied for non-invasive detection and characterization of cells and tissues, showing considerable promise for medical diagnostics and cancer research [58-60]. Pioneering efforts demonstrated that THz pulsed spectroscopy could distinguish healthy from cancerous tissues, including in breast cancer samples [61, 62]. Further research explored how pharmacological treatments alter the terahertz spectral signatures of basal cell carcinomas [63].

Terahertz spectroscopy has also been applied in the detection and analysis of diverse cell types and pathogens, often leveraging its interaction with water molecules despite water's strong THz absorption [11, 58, 59, 64, 65, 66, 67]. To address this limitation, microfluidic devices were developed to enable THz measurements in aqueous environments [68], a technique later refined to resolve biomolecular resonance peaks [69]. Chemometric models combined with THz-TDS have also been used to identify and quantify biomolecules, such as in the quantitative analysis of bovine serum albumin thin films [29, 70], and in the development of label-free DNA detection methods for monitoring hybridization and binding states [71].

Research into bacterial cell components has also advanced significantly. Distinct spectral signatures have been used to differentiate bacterial spores and cells by species or molecular structure [72, 73]. Virus detection is an emerging frontier in which THz-TDS sensing

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techniques are being developed to surpass conventional meta- and nano-sensors in sensitivity for pathogens such as influenza, Ebola, Zika, and SARS-CoV-2 [11, 74].

3.2.3. Advanced spectroscopic characterization of minerals, rocks, and geological systems

The application of THz-TDS to the characterization of minerals, rocks, and geological materials began with early investigations aimed at detecting fundamental physical phenomena through terahertz spectral responses. A foundational study demonstrated that THz-TDS could identify thermally induced electronic spin-crossover transitions in an iron (II) coordination polymer by capturing distinct spectral variations in the 0.1–0.6 THz range, marking the technique's initial use for monitoring subtle structural changes in crystalline systems [76].

In the domain of mineral characterization, THz-TDS has been used to investigate hydrated minerals such as copper sulfate pentahydrate and quartz, revealing absorption coefficients of 5-20 cm^{-1} and refractive indices around 2.1 across the 0.2-2.4 THz range [77]. Moving beyond individual minerals, THz-TDS was applied to both natural and synthetic samples from the Bayan Obo deposit, one of the world's most geologically complex iron oxide and sulfide systems. Measurements in the 0.2-1.3 THz range showed a positive correlation between absorption coefficients, refractive indices, and total iron content (TFe). Binary and ternary mixtures of Fe_3O_4, FeS_2, and Fe_2O_3 were evaluated using random forest regression, achieving average absolute errors below 1% in estimating FeS_2 content. These findings illustrate the potential of THz-TDS, when combined with machine learning, to distinguish minerals with similar compositions and assess their relative abundances for mineralogical exploration and quality control [78, 79].

To address limitations of conventional THz systems, a holographic THz-TDS setup was implemented to characterize 18 representative silicate minerals across the 0.3-3 THz range [80]. This configuration enabled simultaneous acquisition of amplitude, phase, and spectral distribution maps at millimeter-scale resolution. Distinct absorption peaks were identified (such as 1.10 THz for pyrophyllite and 1.15 THz for chamosite), corresponding to specific lattice vibrational modes. Refractive indices ranged from 1.66 to 1.82, and absorption coefficients spanned from 8.25 to 17.68 cm^{-1}, with both parameters reflecting internal structural features and water content.

Rocks, like minerals, present complex internal compositions and structures that influence their dielectric behavior in the terahertz domain. Motivated by the need for automation in mining, researchers applied THz-TDS across the 0.2–2.0 THz range to differentiate coal–rock interfaces [23]. Their work showed that rocks had dielectric constants between 1.75 and 1.87, while coals ranged from 1.56 to 1.74. Coal also exhibited significantly higher absorption coefficients. Using PCA and SVM, classification accuracies reached 100% for rock types and 97.5% for coal types, demonstrating the robustness of THz-TDS for spectral discrimination in complex geologies.

Expanding on this foundation, a subsequent study proposed a more robust methodology for automated, online coal-rock interface characterization [59]. Through analysis of binary mixtures of anthracite and quartz sandstone across the 0.4–2.0 THz range, parametric models were built using BPNN and LSSVM algorithms. These models achieved correlation coefficients above 99% during training and validation accuracies nearing 93%. Estimating cutting drum immersion depth based on rock proportion was also enabled by simulating solid–gas two-

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phase conditions using HDPE. This integration positioned THz-TDS as a quantitative tool for smart mining applications.

A different approach used THz attenuation imaging to generate two-dimensional microporosity maps in carbonate rocks, achieving spatial resolution of 0.5 mm/pixel [81]. This non-invasive method quantified porosity heterogeneity without destructive sampling, enabling mapping of regions with different water retention capacities after saturation, centrifugation, and drying. Cross-validation with standard petrophysical methods confirmed the reliability of the technique, establishing THz-TDS as a viable tool in secondary recovery and petrophysical characterization.

Recent work has extended THz-TDS beyond structural and compositional analysis to geological materials with extended functional roles. For instance, THz-TDS was applied to chloritic schists containing carbonated mica to qualitatively detect effective porosity and calcination products using spectral measurements in the 0.2–1.6 THz range (Yang et al., 2022). Although multivariate models were not employed, the study demonstrated that THz-TDS could non-invasively assess structural and thermal attributes of minerals relevant to energy and medical fields.

In the context of cultural heritage, THz-TDS was applied to stratified geological surfaces such as gypsum and lime in historical frescoes, overcoming geometric distortions and irregularities typically encountered in archaeological samples [82]. Unlike prior research using pressed pellets or idealized sections [53], this study integrated reflection-mode structural imaging with spectral mapping. Self-referenced geometric correction and temporal deconvolution techniques eliminated curvature-induced distortions and isolated internal layer signals, achieving absorption maps at 0.2 mm resolution. The method demonstrated THz-TDS's adaptability to non-invasive analysis of heritage geomaterials for conservation and restoration.

A recent systematic study further demonstrated the capability of THz-TDS for advanced identification of metallic minerals. Sixteen compressed samples of stibnite, sphalerite, galena, and pyrite were evaluated under controlled conditions. Relationships between frequency, concentration, mass, and porosity were established using optical parameters and multivariate algorithms. Cluster analysis based on Euclidean distance allowed classification by lithology, even among minerals with similar compositions, such as galena and stibnite. Strong linear correlations ($R^2 > 0.9$) were observed between frequency and both absorption coefficients and refractive indices, providing a predictive basis for future modeling applications.

These developments illustrate the methodological maturity of THz-TDS as a non-destructive, high-precision spectroscopic platform capable of capturing both localized optical features and multiscale structural variations. The technique is now positioned as a reliable tool for exploration, quality control, mineral reserve estimation, and advanced petrophysical analyses.

3.2.4. Evaluation of liquids and complex chemical mixtures

The application of THz-TDS to liquids began with foundational studies of simple aqueous solutions. In 2001, researchers used dielectric relaxation spectroscopy to investigate how glucose and fructose concentrations affect sub-millimeter water absorption [83]. This was followed by a breakthrough study showing that low-frequency Raman and THz absorption in hydrogen-bonded liquids originates from the same intermolecular vibrational modes, offering a molecular-level view of solvation dynamics [84]. A seminal contribution later consolidated all available measurements of water's complex permittivity over 0-25 THz and 0-100 °C, using physically motivated interpolation functions to provide continuous values for both real and

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imaginary components [85]. The model decomposed the response into three Debye-type relaxations and two Lorentzian resonances, and accurately predicted over 3,100 discrete data points with root-mean-square errors below 5%.

In 2008, researchers revolutionized hydration-shell analysis by applying THz-TDS in ATR geometry. By pressing aqueous solutions against a high-index silicon prism, they created an evanescent THz field that penetrated only a few hundred nanometers into the sample, enabling the direct extraction of interfacial refractive indices and absorption coefficients across 0.2-2 THz [86]. This technique revealed that THz responses scale nonlinearly with solute concentration, indicating extended hydration shells. Monosaccharides were shown to entrain around 10-15 water molecules, disaccharides over 20, and sucrose approximately 35, significantly higher than values from calorimetry, viscometry, or acoustic measurements. These results underscored THz-TDS's unique sensitivity to distal solvent structure.

Later, THz-TDS was extended to probe complex solute-solvent interactions at biological interfaces. In 2011, multilamellar phospholipid membranes under controlled hydration exhibited a sharp absorption feature around 0.7 THz, reflecting sub-picosecond water reorientation near interfaces. This work was expanded in 2014 by studying lipid mixtures undergoing phase transitions, where refractive index and absorption coefficients varied markedly with membrane curvature. Most recently, osmolyte effects on hydration were explored: for example, trehalose reduced water reorientation rates by 40%, shifting THz peaks, while glycerol produced broader spectral damping, both results correlating with protein-stabilizing capabilities.

Parallel applications extended THz-TDS to hydrocarbons and fuels. Distinct broadband absorption fingerprints enabled differentiation between gasoline, kerosene, and diesel [8], while refined oil mixtures were quantified with concentration predictions within 5% using multiparametric analysis [33]. Later studies applied regression techniques for detecting water and glycol contamination in engine oils, achieving sub-percent [87, 88]. Modeling biodiesel-diesel blends as weighted combinations of nonpolar-liquid absorption models, researchers recorded broadband THz spectra (0.5-3.5 THz), estimated fatty acid methyl ester (FAME) content within 3% error, and introduced a simplified dispersion-based indicator for inline quality control [89]. A recent study used principal component analysis and convolutional neural networks to classify 83 crude oil samples by origin, achieving 96.3% accuracy based on THz “fingerprints” linked to asphaltenes and trace metals [90].

In pharmaceutical and biofluid analytics, THz-TDS has recently enabled non-invasive, real-time quantification of active pharmaceutical ingredients (APIs). One study combined THz-TDS with a convolutional neural network to analyze anti-tuberculosis fixed-dose formulations over 0.3–1.5 THz, achieving <3% error in sub-minute process control [91]. Beyond small molecules, THz-TDS has been used to study complex biomolecular solutions through effective-medium theories. For example, Debye–Lorentz modeling of bovine serum albumin suspensions isolated hydration-shell contributions and estimated shell thicknesses of 1–2 nm [29]. Similar models mapped hydration dynamics in peptide mixtures with sub-picosecond resolution [92]. Studies of trehalose solutions also revealed hydration numbers near 15 and shells extending beyond 0.5 nm, validated through Maxwell–Garnett and Bruggeman formalisms [93].

Together, these studies demonstrate that THz-TDS, when integrated with effective-medium theories such as Maxwell–Garnett, Bruggeman, and Looyenga, can decompose total permittivity into contributions from bulk water, hydration shells, and macromolecular cores. From this decomposition, shell thicknesses, volume fractions, and dielectric contrasts can be

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quantified directly from frequency-dependent THz data, highlighting the method's powerful potential for non-destructive analysis of liquids and chemically complex systems.

This review critically assesses the application of THz-TDS for material characterization, aligning its findings with the research objectives outlined earlier. The discussion begins by situating the extracted insights within the broader scientific literature, highlighting key contributions, recurring methodological patterns, and points of divergence. From this comparative synthesis, we develop a unified conceptual framework that integrates the principal methodological and analytical approaches observed across studies. We then explore the theoretical, practical, and regulatory implications of THz-based material probing, while also identifying technical and procedural limitations reported in the literature. Finally, we propose future research directions aimed at deepening the understanding of THz–matter interactions and expanding the applicability of this technique across emerging domains.

The predominance of THz-TDS applications in semiconductors, optical substrates, and polymeric films underscores the technique's unique capacity to probe charge-carrier dynamics and dielectric properties without altering material structure. This trend aligns with recent developments, such as the 8×8 photoconductive antenna array that enables high-resolution, spatially resolved terahertz imaging [94], and the early introduction of reflection-mode THz-TDS for substrate-sensitive measurements [95]. Notably, over 40% of the studies included in this review employed transmission-mode THz-TDS to extract refractive indices and absorption coefficients, particularly in advanced materials such as graphene and manganite thin films [18].

In recent years, THz-TDS has undergone substantial advancements that have significantly improved its utility in materials characterization, as illustrated in **Figure 7**. **Figure 7** presents a synthesis of recent advances that have significantly enhanced the performance of terahertz spectroscopy for material characterization. The figure was compiled by the authors based on peer-reviewed studies indexed in Scopus and Web of Science. One major development is the growing use of the Drude-Smith model to describe non-Drude transport behavior in materials with localized carriers or backscattering effects. This modeling approach has been applied effectively to correlated oxides and graphene [18, 38]. These studies emphasize the critical importance of selecting appropriate physical models when interpreting terahertz conductivity. In particular, the integration of oblique-incidence reflection-mode measurements with a generalized Drude-Smith framework was shown to enhance sensitivity to substrate-induced effects, further validating the use of reflection-mode geometries in systems where transmission is impractical [38].

A major area of progress involves the integration of computational simulation techniques, particularly density functional theory (DFT), which enables theoretical validation of observed spectral features. This approach has been successfully employed to correlate absorption bands with specific vibrational modes and crystalline structures [96, 97]. In parallel, new modeling strategies have been proposed to simplify data interpretation. For instance, a recent study introduced an analytical model that treats ultrathin films as conductive sheets, thereby improving sensitivity at the nanoscale [98].

Additional methodological advances have centered on optimizing parameter extraction and improving spectral resolution. Statistical and machine learning techniques, such as principal component analysis (PCA) and support vector machines (SVMs), have enabled automated classification of complex materials in real time [23]. Interval partial least squares (iPLS) can enhance the selection of relevant spectral regions, leading to more accurate predictions. Expanding the detection bandwidth has also played a crucial role; measurements up to 170 THz have been reported, greatly extending the range of analyzable materials [21].

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The refinement of THz spectroscopy has also been driven by efforts to identify and control key variables that impact spectral resolution, sensitivity, and the accuracy of extracted optical parameters. The choice of physical model remains critical. While the classical Drude model is appropriate for metallic systems, the Drude–Smith extension better captures the behavior of materials with backscattering or partial carrier localization [20]. Similarly, the selection between reflection and transmission modes directly influences spectral quality. In anisotropic materials, combining reflection-mode setups with polarization control has been shown to yield more accurate dielectric profiles [16]. Moreover, ultrashort-pulse laser sources have extended the available spectral bandwidth, enabling the detection of higher-frequency vibrational modes [96].

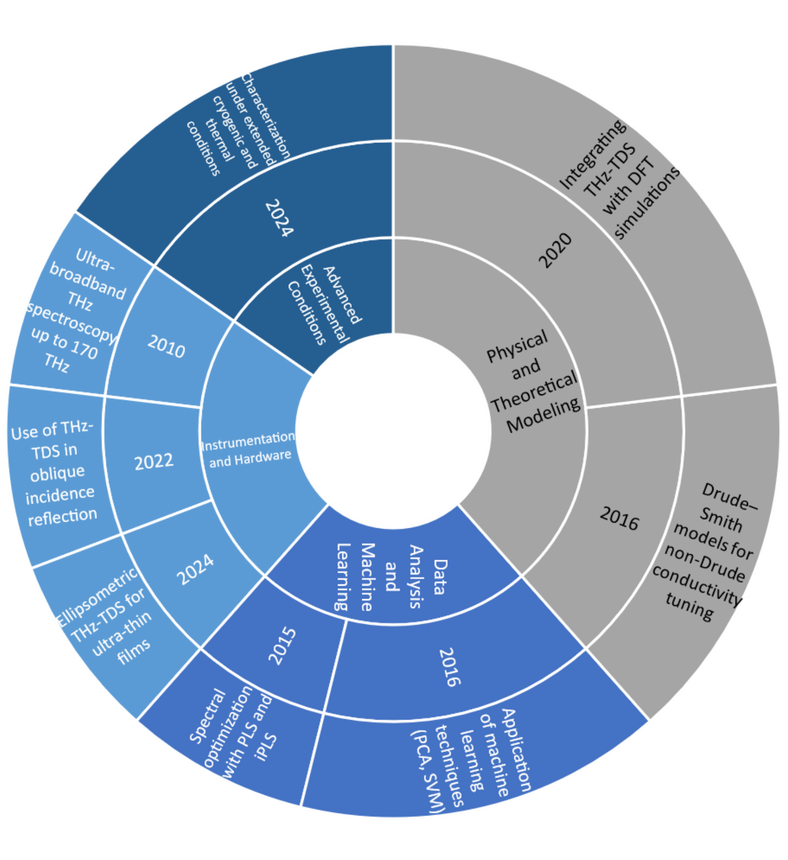

Figure 7. Recent advances that have enhanced the performance of terahertz spectroscopy for material characterization. Compiled by the authors based on data from Scopus and Web of Science.

Environmental and experimental variables also significantly affect THz system performance. Precise sample holder design and optical alignment have been shown to reduce phase noise and improve signal-to-noise ratios [95]. Likewise, ambient humidity introduces water vapor absorption artifacts that can distort spectra; mitigation strategies such as nitrogen-purged chambers have been advocated to address this challenge [99]. In terms of data analysis, statistical tools like PCA and partial least squares regression (PLS) have proven effective in enhancing classification accuracy and automating the selection of discriminative spectral regions [100]. These experimental and computational variables are synthesized in **Figure 8**, which outlines representative strategies for improving spectral fidelity and analytical precision across diverse material classes. The figure captures the interplay between

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measurement geometry, data preprocessing, model selection, and environmental control, each of which contributes to the accuracy and reproducibility of terahertz spectroscopic measurements.

Building upon the synthesized results presented in this review, **Figure 9** introduces a conceptual model for material characterization using terahertz spectroscopy. This model integrates the core functional stages required for the acquisition, processing, and analysis of spectroscopic data aimed at accurately identifying physicochemical and structural material properties. The THz-based characterization pipeline is structured into six key phases.

(i) First, sample preparation involves selecting the appropriate material state (solid, liquid, or thin film) and controlling key variables such as sample thickness, temperature, and environmental conditions [80]. Second, data acquisition is conducted using either a THz-TDS or THz-CW system, with careful consideration of the measurement geometry (transmission, reflection, or ATR) to match the sample type and expected optical response [41, 101].

(ii) In the signal processing phase, the time-domain signal is transformed into the frequency domain using the fast Fourier transform (FFT), followed by baseline correction and normalization steps. This enables the calculation of fundamental optical parameters such as the refractive index, absorption coefficient, and complex permittivity. These parameters are then modeled using theoretical frameworks like the Drude–Lorentz model or density functional theory to extract meaningful physical insights [96].

(iii) In the analytical enhancement phase, complementary characterization techniques such as FTIR, SEM, or differential scanning calorimetry may be integrated to validate or enrich the THz findings. Additionally, machine learning algorithms (such as principal component analysis (PCA), support vector machines (SVM), and neural networks) are often employed to improve data interpretation and enable classification or regression tasks in complex datasets [27].

(iv) Finally, in the interpretation stage, the computed parameters are contextualized to derive structural, electrical, or functional characteristics of the sample. These outputs inform materials evaluation in various fields, including semiconductor diagnostics, pharmaceutical quality control, biofluid analysis, and mineral exploration [102].

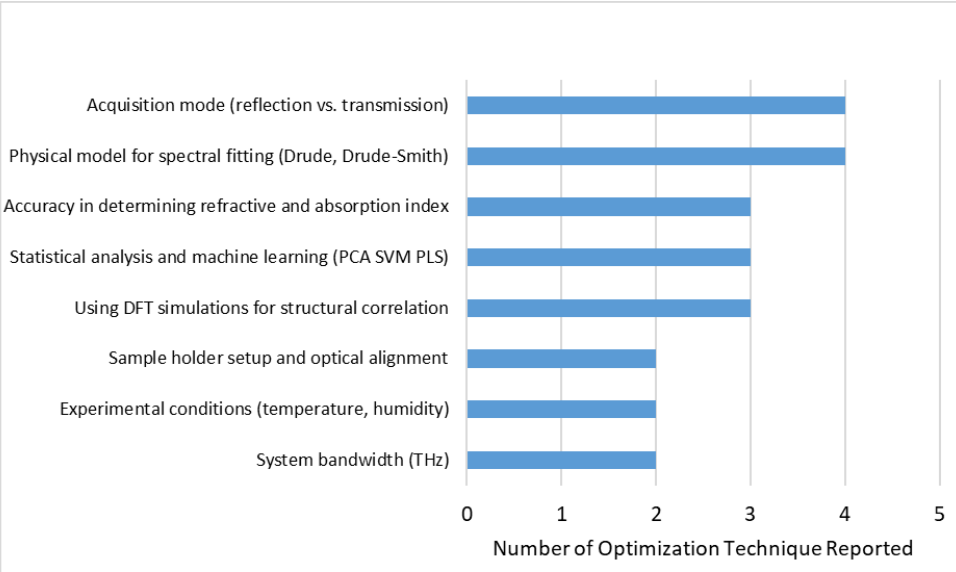

Figure 8. Variables associated with the optimization of terahertz spectroscopy for material characterization. Compiled by the authors based on data from Scopus and Web of Science.

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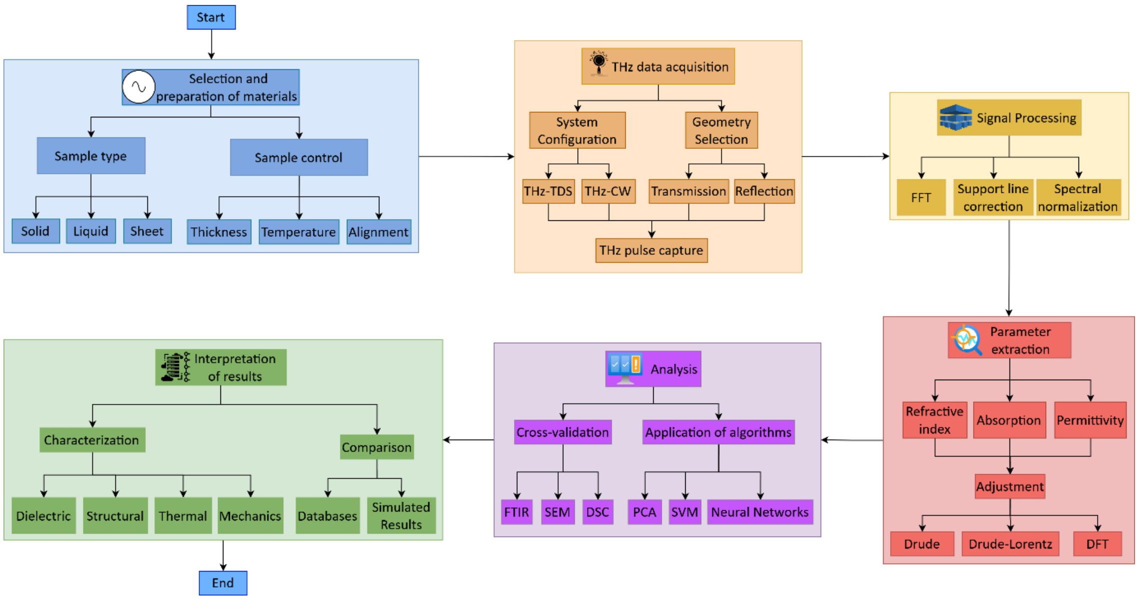

Figure 9. Operational model for material characterization using THz spectroscopy. Compiled by the authors based on data from Scopus and Web of Science using Draw.io.

3.3. Comparison of Findings with Other Studies

The results of this review support and expand upon the methodological diversity observed in the THz-TDS literature, where acquisition geometry, theoretical modeling, and data analytics are tailored to specific material properties and application requirements. Early transmission-mode studies in liquid dielectrics and biological tissues demonstrated sub-percent sensitivity to changes in refractive index and water content [15, 103]. Similarly, the integration of quartz-wedge polarimetry into a reflection-mode system significantly improved the characterization of anisotropic materials [16]. These studies underscore the importance of choosing between transmission, reflection, polarimetry, or ellipsometry based on sample transparency, geometry, and optical interaction.

Recent research has advanced toward hybrid, multiparametric frameworks. For example, density functional theory (DFT) simulations have been used in conjunction with spectral data to identify absorption bands in antioxidant-functional polymers [104]. The fusion of ellipsometry, differential scanning calorimetry, and terahertz spectroscopy has revealed shifts in complex permittivity linked to glass transitions in polymer systems [105]. Similarly, porosity mapping in composite membranes has been enhanced using effective-medium models, mercury porosimetry, and impedance spectroscopy [106]. These integrative approaches validate and refine THz-derived metrics through complementary methodologies.

Beyond classical optical constants (such as refractive index, absorption coefficient, and permittivity), THz-TDS now probes structural, thermal, and functional properties. For instance, concepts like "THz coloration" and holographic imaging have revealed linear correlations between THz optical signatures and crystallographic parameters for mineral classification [80]. Advanced signal processing methods, including ensemble empirical mode decomposition (EEMD) and long short-term memory (LSTM) neural networks, have been applied to raw time-domain waveforms to detect subsurface corrosion with sensitivities exceeding those of traditional spectral analysis [78]. In food science, THz spectroscopy has also been used to identify lipid polymorphs for traceability and quality control [107].

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Time-resolved optical pump/THz-probe spectroscopy has further enabled the investigation of ultrafast carrier and lattice dynamics on femtosecond to picosecond timescales [108]. For instance, dual-timescale charge-carrier relaxation in perovskite materials was observed using this technique, revealing both sub-200 fs and 2 ps decay components [109]. Meanwhile, scattering-type near-field optical microscopy (s-SNOM) combined with THz-TDS has achieved lateral resolutions of about 170 nm, enabling quantitative hyperspectral nano-imaging of local carrier concentrations. A 40×20-pixel image covering 0.4-1.8 THz was collected over 180 minutes, with Drude-model fitting applied to each pixel.

Flexible metamaterial resonators have also increased THz sensitivity at ultralow concentrations. For example, split-ring resonator arrays have achieved nanomolar or picomolar detection limits in pesticide sensing, including stable detection of chlorpyrifos methyl at about 130 ppb on fruit surfaces, even after 1000 bending cycles [110]. These results point to the simplicity, adaptability, and robustness of THz-TDS platforms in chemical sensing.

Finally, artificial intelligence, quantum modeling, and calibrated spectrum analysis are emerging as powerful tools to enhance the precision and scalability of THz applications. Quantitative material characterizations have been achieved through machine-learning models such as partial least squares regression (PLSR), random forests, and multilayer perceptrons (MLP), applied to diverse polymer blends [19]. Similarly, phase-transition detection in clay minerals has been enabled by integrating thermal analysis with THz spectroscopy. These trends clearly signal a shift toward data-driven, multiparametric THz-TDS workflows for high-accuracy material characterization.

3.4. A Conceptual Framework Proposal

A robust conceptual framework for future THz-TDS research in material characterization must integrate infrastructure realities, methodological rigor, and scalable data practices, as illustrated in **Figure 10**. In many developing research regions (including Latin America and sub-Saharan Africa), the absence of high-resolution THz instrumentation hampers throughput and limits adoption. Addressing this requires shared facilities, portable sensor platforms, and regional training programs. In parallel, geological characterization efforts in Central Asia and the Andean region necessitate spectrum libraries and field-adapted protocols tailored to local mineralogical profiles [19]. In hyper-humid zones like Southeast Asia and the Amazon, real-time atmospheric correction algorithms and robust environmental controls are essential to manage water vapor absorption and preserve spectral accuracy [104].

At its core, the framework emphasizes rigorous model selection, calibration, and uncertainty propagation. Fitting procedures should include Drude-Smith, Debye-Lorentz, effective-medium approximations, and first-principles DFT simulations, validated through standardized goodness-of-fit metrics [38, 96]. Cross-validation using complementary techniques such as SEM, XRD, or Raman spectroscopy is necessary to resolve overlapping features in structurally complex materials [105]. Advanced machine-learning pipelines (including ensemble regressors, convolutional neural networks, and transformer-based models) enable high-throughput analysis, classification, and anomaly detection in multidimensional THz datasets [24, 106].

To promote reproducibility and interoperability, the framework calls for open-access, region-specific THz spectrum libraries adhering to FAIR data principles. These libraries should align with global geoscience initiatives such as Deep-Time Digital Earth and include metadata covering sample origin, ambient conditions, and instrument parameters [95]. Quantifiable metrological benchmarks (such as detection limits, spectral and spatial resolution, and

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penetration depth) must also be established to support claims of non-destructivity and to form the basis for emerging industry standards [107].

In the broader innovation ecosystem, THz-TDS must integrate with application domains such as infrastructure monitoring, pharmaceutical production, and environmental diagnostics. This requires interoperable sensor networks, real-time data analytics, and digital-twin frameworks for predictive maintenance and decision support. Sustained progress will depend on public-private partnerships, regional consortia, and targeted capacity-building efforts to ensure equitable, technically rigorous advancement of THz technology across scientific, industrial, and policy landscapes.

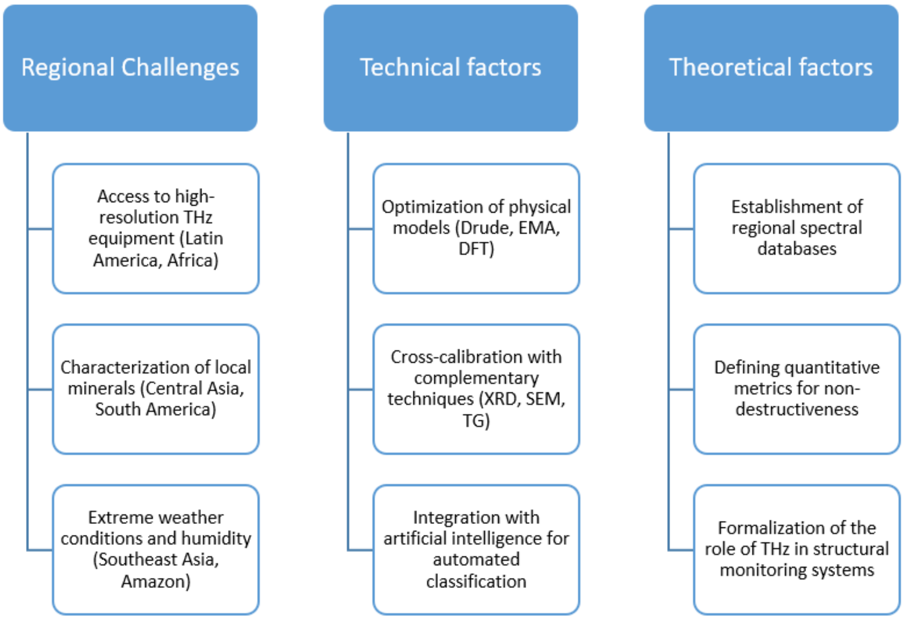

Figure 10. Proposed conceptual framework for THz-TDS–based material characterization, developed in-house from analyses of Scopus and Web of Science data.

3.5. Implications, Limitations, and Future Research

THz-TDS's versatility as a non-contact, non-destructive probe has made it increasingly valuable across industrial and scientific domains. In semiconductor manufacturing, THz-TDS enables wafer-scale mapping of electrical properties (such as carrier density, mobility, and conductivity) with sub-millimeter spatial resolution, providing a rapid, non-invasive alternative to conventional four-point probing for in-line quality control [41].

Beyond semiconductors, THz-TDS has been effectively used to assess surface roughness and topography in complex metallic geometries. Reflection-mode measurements on 3D-printed stainless-steel components have shown good agreement with laser-scanning microscopy, demonstrating its potential for contactless inspection in aerospace and biomedical manufacturing [102].

Recent developments in coating metrology have eliminated the need for prior knowledge of the refractive index. For example, the portable PHASR Scanner employs a polarimetric THz system, sparse deconvolution, and a physics-based linear model to measure multilayer CFRP coating thickness with a root-mean-square error of less than 10 µm and greater than 92% accuracy on optically opaque substrates. This system, trained using machine learning, is especially suited for in-line industrial metrology.

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Additionally, THz-TDS has demonstrated strong potential in challenging environments, including high humidity and industrial harshness. A reflection-mode system enhanced by backpropagation neural networks was shown to visualize coating thickness on steel plates without requiring prior knowledge of material refractive indices [27]. This method not only generates high-resolution thickness maps but also detects localized defects (such as scratches or inclusions) while simultaneously extracting material-specific optical parameters. These capabilities position THz-TDS as an indispensable tool for real-time quality assurance in sectors like aerospace, construction, biomedical devices, and electronics manufacturing, where rapid and accurate assessment of multilayer coatings is essential for durability and operational efficiency.

Despite its strengths, THz-TDS faces several persistent limitations that must be addressed to enable widespread industrial deployment.

(i) Sensitivity to experimental and environmental conditions remains a major concern. Minor misalignments or deviations in sample thickness (<100 µm) can cause significant phase and amplitude distortions. Moreover, residual water vapor can mask weak spectral features, as shown in studies on aqueous samples [103]. Even the selection of window functions during Fourier transformation has been shown to induce up to 10% variation in refractive index retrieval, depending on the specific algorithm used [111].

(ii) Modeling limitations hinder accurate parameter extraction. Conventional Fresnel-based inversion fails in ultrathin films (<1 µm) due to interference and dispersion effects. Without advanced hybrid frameworks (such as Drude-Smith-Fresnel or ellipsometric models), errors in estimating carrier density and conductivity can exceed 20% [112].

(iii) Challenges in generating and detecting stable THz pulses (especially in the low-frequency range (< 0.3 THz)) limit resolution in critical spectral regions where biomolecular fingerprints reside. Instability in pump-laser timing, antenna bias, and detector response contributes to poor signal-to-noise ratios in this range [113].

(iv) A lack of reproducibility and standardization across laboratories impedes data consistency. While initiatives like dotTHz aim to unify data formats and processing tools, they are not yet universally adopted. A recent interlaboratory comparison across 15 facilities reported up to 15% variation in retrieved optical constants for identical samples, highlighting the urgent need for shared calibration standards and harmonized protocols.

(v) A systematic framework for propagating uncertainties across the entire measurement pipeline (from time-domain signal acquisition to material parameter estimation) is still in early development. Despite initial efforts to characterize both random and systematic errors in THz-TDS, no unified uncertainty quantification methodology has been established [114]. Overcoming these limitations is essential for transitioning THz-TDS from a research tool to a robust industrial metrology platform.

As THz-TDS matures, four synergistic research frontiers are emerging that promise to redefine its capabilities:

(i) The characterization of ultrathin and high-critical-temperature (high-Tc) superconducting films is driving innovation in cryogenic pump–probe and magneto-THz techniques. For example, researchers have studied carrier dynamics in superconducting films using these methods, laying the groundwork for applications in materials such as $YBa_2Cu_3O_{7-x}$ and FeSe monolayers [98]. Dual-timescale optical-pump/THz-probe measurements have revealed both sub-200 fs and 2 ps charge-carrier relaxation components in $CH_3NH_3PbI_3$ perovskites [27], while gapless superconductivity in Nb thin

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films was mapped under in-plane magnetic fields [115]. Extending these approaches to high-Tc systems will require enhanced signal-to-noise ratios, precise polarization control, and millikelvin-level thermal stability.

(ii) Hybrid multilayer metrology platforms are being developed to analyze complex stratified materials in a single scan. Integrating complementary split-ring resonators with homodyne detection enables frequency-selective imaging of individual layers within metamaterial stacks [101]. Future systems should combine time- and frequency-domain detectors, automated scanning, and adaptive windowing algorithms to extract interfacial permittivity and layer-specific composition.

(iii) Artificial intelligence is reshaping THz spectroscopy into an autonomous sensing modality. Backpropagation neural networks have already demonstrated >96% accuracy in predicting coating thickness on steel plates, even in the absence of refractive index inputs [27]. The future lies in coupling THz inversion engines with physics-informed neural networks, deep ensembles, and Bayesian uncertainty models to enable real-time waveform interpretation, sub-micrometer resolution, and automated detection of delamination, voids, and inclusions.

(iv) Metamaterial-enhanced sensors are driving ultra-sensitive detection in environmental, agricultural, and food safety contexts. For instance, flexible split-ring resonators have enabled pesticide detection at concentrations as low as 130 ppb, maintaining stability even after 1000 bending cycles [110]. These advances mark the convergence of THz engineering, nanophotonics, and materials science, pointing toward deployable, high-precision THz sensors.

The results obtained from this systematic literature review demonstrate that THz-TDS has consolidated its position as a high-resolution, non-contact analytical tool capable of accurately characterizing structural, optical, and dielectric properties across a wide variety of materials. Through the analysis of 25 primary studies guided by the PRISMA 2020 methodology, significant methodological advancements were identified, including multiscale spectral modeling (e.g., Drude–Smith, Debye–Lorentz), the integration of artificial intelligence algorithms (PCA, SVM, CNN), and the development of experimental architectures that overcome traditional limitations in temporal and spectral resolution.

The identified applications range from dielectric mapping in semiconductors and the characterization of rocks and minerals using holographic techniques and spectral classification, to the non-invasive analysis of biological solutions, pharmaceutical cocrystals, and biomaterials. Industrial metrology has also seen important developments, such as the use of neural networks for the automated quantification of metallic and polymeric coating thickness. Although the technique has shown remarkable versatility, its broader industrial adoption remains limited by technical and practical challenges, including humidity sensitivity, dependence on specific geometries, lack of interlaboratory calibration protocols, and the absence of formal uncertainty estimates. Nevertheless, hybrid approaches combining spectroscopy and computational modeling, along with the advancement of portable platforms and the implementation of open standards such as dotTHz, suggest a promising outlook for its deployment in strategic sectors such as mining, pharmaceuticals, heritage conservation, and advanced manufacturing.

Furthermore, the review reveals that THz-TDS is no longer restricted to simple or homogeneous materials; it has demonstrated the capacity to analyze complex, stratified, or porous structures, such as those found in carbonate rocks, ultrathin films, and archaeological

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surfaces. Regarding gaps in the literature, a notable lack of cross-validation using complementary techniques (FTIR, NMR, SEM) was identified, which limits the reproducibility of the reported optical parameters. The systematic incorporation of external verification methods and uncertainty estimation would strengthen reliability and broaden acceptance of this technology. Finally, the findings suggest that the versatility of THz-TDS is significantly enhanced when integrated with computational models and deep neural networks, enabling its use as an autonomous sensor in intelligent mining environments, pharmaceutical quality control, and in situ analysis of cultural heritage materials.

4. CONCLUSION

This review confirms the versatility of terahertz time-domain spectroscopy (THz-TDS) as a high-resolution, non-contact tool for characterizing structural, optical, and dielectric properties across various materials. Applications span semiconductors, minerals, pharmaceuticals, and biomaterials. Methodological advances (such as AI integration and hybrid modelling) enhance analytical precision. However, challenges remain, including humidity sensitivity, lack of standardization, and limited uncertainty quantification. The technique's effectiveness in analyzing complex and stratified materials highlights its growing potential. Future progress depends on portable systems, open data standards, and cross-validation protocols. THz-TDS is poised to become a key platform in smart manufacturing and scientific exploration.

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6. AUTHORS' NOTE

The authors declare that there is no conflict of interest regarding the publication of this article. Authors confirmed that the paper was free of plagiarism.

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