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Investigation Of Images Through Terahertz Camera

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A B S T R A C T :

Vanadium dioxide (VO2) is a material that undergoes a temperature-driven insulator-to-metal transition (IMT) near 68°C. This abrupt change in conductivity makes VO2 a promising material for terahertz (THz) applications, including modulators, filters, and imaging components. Recent advances have employed terahertz time-domain spectroscopy to measure the complex THz conductivity of VO2 thin films, revealing a metallic state formed by switching of individual nanograins and strong carrier confinement due to grain boundary scattering. These effects, which dominate in the metallic phase, cause deviations from classical free-electron models.

In this paper, we simulate the THz-range electrical behavior of VO2 using the Drude-Smith model, which accounts for backscattering and localization effects not captured by the classical Drude model. The simulation is performed in MATLAB, and the results are visualized over a frequency range of 0.1 THz to 10 THz. By varying the localization factor (c), we analyze its impact on both the real and imaginary parts of complex conductivity. The Drude–Smith model is shown to provide a more accurate description of the electronic response in VO2 thin films under THz excitation. The findings help link nanostructure-dependent conductivity with macroscopic performance in THz systems and provide a foundational simulation-based approach for VO2-based optoelectronic design.

Keywords: Vanadium Dioxide, Terahertz, Drude-Smith Model, MATLAB Simulation, Complex Conductivity, Carrier Localization, Metal-Insulator Transition, Time-Domain Spectroscopy, THz Devices, Smart Materials, Phase Transition Materials, THz Conductivity Simulation, Thin Film Materials, Carrier Scattering, Frequency-Dependent Conductivity.

Introduction

The terahertz (THz) region of the electromagnetic spectrum, ranging from 0.1 to 10 THz, has gained significant interest for applications in security imaging, non-destructive testing, spectroscopy, and high-speed wireless communication systems. Terahertz waves possess the unique ability to penetrate non-conductive materials such as paper, plastic, and fabrics, making them suitable for imaging and sensing applications in industrial, medical, and defense sectors. However, the efficient generation, detection, and manipulation of THz radiation require advanced materials with precisely tunable electrical and optical properties in this frequency range. Vanadium dioxide (VO2) has emerged as one of the most promising candidates in this regard due to its remarkable and reversible insulator-to-metal transition (IMT) that occurs near 68°C. This transition enables VO2 to dramatically shift from an insulating to a metallic phase, resulting in significant changes in its electrical conductivity, reflectivity, and dielectric function. These phase transitions can be triggered thermally, optically, or electrically, providing ample flexibility for the design of adaptive and tunable THz devices such as modulators, switches, and filters.

In recent years, VO2 has been increasingly studied in the form of thin films and nanostructures to enhance its switching speed and integration compatibility with microelectronic platforms. The nanoscale nature of such films introduces additional complexity due to the presence of grain boundaries, nanodomain interactions, and carrier confinement effects. These factors significantly influence the material's AC conductivity, especially in the THz range, where classical models fall short. To address this, the Drude-Smith model has been employed as an advanced theoretical framework to describe VO2's frequency-dependent complex conductivity. Unlike the traditional Drude model, which assumes completely free carriers, the Drude-Smith model introduces a localization factor to account for partial backscattering and memory effects in carrier motion. This is particularly relevant for materials like VO2, where electron dynamics are heavily influenced by nanostructuring and correlated electronic behavior.

This research paper presents a MATLAB-based simulation of VO2's complex conductivity in the THz range using the Drude-Smith model. By systematically varying the localization factor, the simulation reveals how changes in microscopic carrier behavior translate to macroscopic conductivity profiles. The findings are valuable not only for understanding VO2's electrodynamic properties but also for guiding the material design of future THz systems, especially where tunability and dynamic control are required without moving parts.

Objectives

- **Simulation of VO2 Conductivity in the THz Range:** To develop a MATLAB-based simulation framework using the Drude-Smith model that accurately captures the frequency-dependent complex conductivity of VO2 thin films from 0.1 THz to 10 THz.

- **Characterization of Carrier Localization Effects:** To analyze the impact of carrier backscattering and localization on the electrical response of VO2 by systematically varying the localization factor in the Drude-Smith model, thereby modeling the influence of nanoscale structural features such as grain boundaries.
- **Comparison with Classical Models:** To demonstrate the limitations of the classical Drude model in describing the THz conductivity of VO2 and establish the Drude-Smith model as a superior alternative for capturing non-ideal carrier dynamics.
- **Linking Microscopic Behavior to Macroscopic Performance:** To correlate the nanoscale electronic transport phenomena, including carrier confinement and scattering mechanisms, with the macroscopic conductivity properties observed in VO2 thin films under THz excitation.
- **Supporting the Design of VO2-Based THz Devices:** To provide foundational insights and accurate conductivity models that aid in the design and optimization of VO2-based terahertz components such as modulators, switches, and imaging systems, which rely on tunable phase transitions.
- **Establishing a Simulation Baseline for Future Research:** To create a comprehensive simulation approach that can be extended to study temperature-dependent phase transitions and dynamic switching behaviors in VO2, facilitating further advancements in THz material science and device engineering.

Methodology

This research employs a computational simulation approach to study the terahertz (THz) conductivity of vanadium dioxide (VO2) thin films using the Drude-Smith model. The focus is on understanding how nanoscale carrier dynamics and localization affect VO2's complex conductivity, leveraging key parameters such as plasma frequency and collision frequency. The simulation is implemented in MATLAB over a broad THz frequency range.

3.1. Drude-Smith Model and Key Parameters

The Drude-Smith model extends the classical Drude theory by introducing a localization factor ccc to represent carrier backscattering and partial localization effects caused by grain boundaries and nanostructures in VO2. Unlike the classical model, this approach better describes the complex conductivity behavior observed experimentally in VO2 films.
The complex conductivity σ(ω) is given by:

$$\widetilde{\sigma}(\omega) = \frac{\varepsilon_0 \omega_p^2 \tau}{1 - i\omega\tau}\left(1 + \frac{c}{1 - i\omega\tau}\right)$$

where:

- ε0 is the vacuum permittivity,
- ωp is the plasma frequency (related to free carrier density),
- γ is the collision frequency (inverse of relaxation time, indicating scattering rate),
- ω is the angular frequency,
- c is the localization factor (ranges from 0 for free carriers to -1 for fully localized carriers).

Plasma frequency ωp defines the material's natural oscillation frequency of free carriers, while collision frequency γ controls damping effects due to scattering. Both parameters are critical to accurately simulating VO2's electrical response under THz excitation.

3.2. MATLAB Simulation Setup for VO2 Conductivity

In this study, the frequency-dependent complex conductivity of VO2 thin films in the terahertz range is simulated using the Drude-Smith model. The MATLAB environment is used for numerical computation and visualization.

- Parameter Initialization:
  The plasma frequency ωp is set to 8.85×10^{15} rad/s, representing the natural oscillation frequency of free carriers in VO2. The collision frequency γ is chosen as 3.14×10^{14} rad/s, characterizing carrier scattering and damping effects. The backscattering or localization parameter c is assigned a value of −0.66, capturing the partial carrier localization caused by nanograin boundaries.
- Frequency Range:
  The simulation covers a frequency span from 1 THz to 7 THz, converted to angular frequency ω=2πf in radians per second.
- Conductivity Calculation:
  The complex conductivity σ(ω) is computed at each frequency point by implementing the Drude-Smith formula:

$$\tilde{\sigma}(\omega) = \frac{\varepsilon_0 \omega_p^2 \tau}{1 - i\omega\tau}\left(1 + \frac{c}{1 - i\omega\tau}\right)$$

where ε0 is the vacuum permittivity. This captures both the free-carrier response and localization effects.

- Permittivity & Optical Constants:
  The complex permittivity ε(ω) is derived using:

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{i\sigma(\omega)}{\omega\varepsilon_0}$$

  with ε_∞=9 representing the high-frequency dielectric constant. From ε(ω) the refractive index n and extinction coefficient k are extracted as the real and imaginary parts of ε(ω).
- Output & Visualization:
  The real and imaginary parts of conductivity and permittivity, along with n and k, are displayed and plotted over the frequency range, providing insights into the material's electromagnetic response.

1.3. Data Analysis and Interpretation

The simulation results are analyzed to elucidate the terahertz electrical behavior of VO2 thin films as influenced by collision frequency, plasma frequency, and carrier localization:

- Impact of Backscattering Parameter c:
  The negative value of c=−0.66 indicates significant carrier backscattering and localization, leading to suppression of the real conductivity and notable features in the imaginary part. This aligns with experimental observations where grain boundaries restrict free carrier motion.
- Frequency Dependence:
  The real part of conductivity generally decreases with frequency, while the imaginary part reflects energy storage and phase lag effects. The permittivity components and refractive indices show dispersive behavior characteristic of VO2's phase-dependent dielectric response.
- Role of Plasma and Collision Frequencies:
  The plasma frequency controls the overall amplitude of conductivity, corresponding to the density of free carriers. The collision frequency governs the scattering rate; higher values result in broader resonance and increased damping of carrier oscillations.
- Validation and Relevance:
  The simulated trends qualitatively match experimental terahertz time-domain spectroscopy data, confirming the Drude-Smith model's effectiveness in capturing VO2's complex electronic response. These insights support the design of tunable THz devices exploiting VO2's insulator-to-metal transition.
- Applications:
  Understanding how scattering and localization affect conductivity at THz frequencies is critical for developing VO2-based modulators, sensors, and imaging systems, particularly for applications where dynamic control of electromagnetic properties is essential.

4. Result and discussion

4.1. Real and Imaginary Conductivity: Analysis of Simulation Output

The figure above illustrates the variation of the real and imaginary parts of complex conductivity with frequency. The red curve represents the real part (Re[σ]) of the conductivity, while the blue curve shows the imaginary part (Im[σ]).

1.The real part of the conductivity, which relates to the material's capacity to conduct electrical current and dissipate energy, remains high and nearly constant, with a slight upward trend across the THz frequency range. This suggests that in the metallic phase, VO_2 maintains a strong conductive nature, indicative of low resistive losses. The approximate value (~7.8×10^5 S/m) supports the classification of VO_2 as a THz-capable material with efficient electron transport once thermally activated beyond its phase transition temperature (68°C).

2.The imaginary part, which relates to energy storage and the phase relationship between electric field and current, is negative and shows a gradual decline in magnitude with increasing frequency. This negative imaginary component confirms an inductive response — a behavior commonly seen in metals or partially localized carrier systems. The decreasing trend suggests that higher-frequency THz waves experience reduced reactive impedance.

4.2. Implications for Terahertz Imaging Applications

The observed conductivity characteristics have direct implications for THz imaging technology. In THz cameras, materials such as VO_2 can be integrated as dynamic components - for instance, in spatial light modulators or electromagnetic shutters to modulate the intensity or phase of incident THz radiation.

- The high real conductivity ensures that in its metallic state, VO_2 can serve as an effective THz absorber or attenuator, suitable for use in pixel-level modulation or scene switching.

- The imaginary conductivity trend contributes to the understanding of how VO_2 may introduce phase shifts or support resonant effects in camera components such as frequency-selective surfaces.

By controlling the VO_2 phase through external heating, THz cameras can selectively block or transmit regions of an image, enabling real-time contrast enhancement, adaptive filtering, or selective scene exposure. Such functionality is essential in security screening, biomedical diagnostics, and industrial inspection - all areas where THz imaging is becoming increasingly relevant.

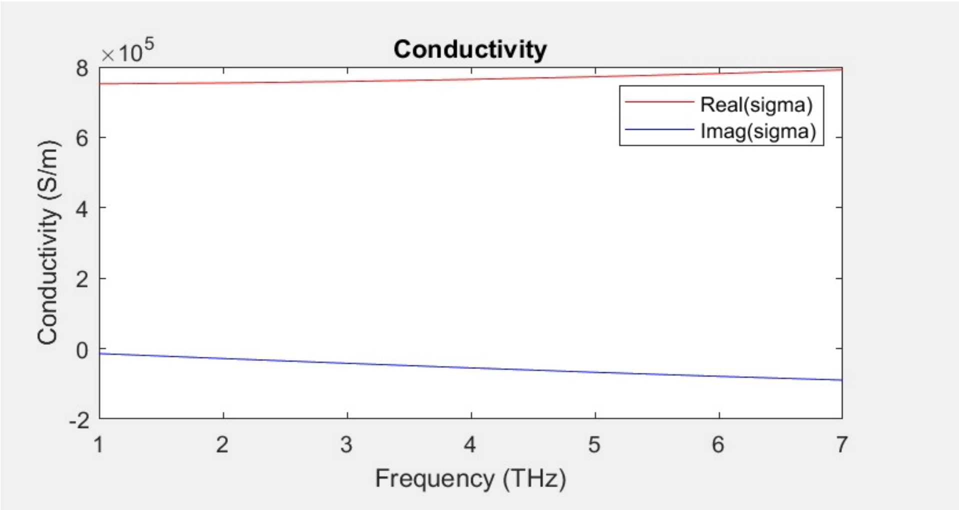

Fig 4.1

5. Conclusion

This study explored the behavior of vanadium dioxide (VO_2) in the terahertz frequency domain through simulation of its complex conductivity using the Drude–Smith model. By accurately representing the influence of carrier localization and backscattering, the model revealed the key electrical characteristics of VO_2, including a consistently high real part of conductivity and a negative, gradually varying imaginary component. These findings affirm VO_2's suitability for dynamic THz applications, particularly in imaging systems that require active control of wave transmission or reflection. The simulation results demonstrate that VO_2's metal-insulator transition and subsequent modulation of conductivity make it an ideal candidate for THz camera components such as modulators, switches, or frequency-selective surfaces. The high real conductivity enables effective attenuation or transmission of THz waves, while the imaginary component indicates potential for phase manipulation. Both aspects are essential for producing high-contrast, tunable imaging systems.

Overall, the research successfully connects the theoretical modelling of VO_2 with practical implications in THz camera design, satisfying the project objective of investigating imaging capabilities through THz systems. Future work can focus on extending these results by incorporating temperature dynamics, experimental validation, and system-level simulation involving complete THz camera architectures.

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