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Comparative Analysis of Classical and Modified Classical Dielectric Function Models for Semiconductor Characterization: A Comprehensive Study

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Abstract

This comprehensive study presents a detailed comparison between Classical Dielectric Function (CDF) and Modified Classical Dielectric Function (MDF) models for semiconductor characterization through infrared reflectance spectroscopy. The analysis encompasses mathematical formulations, accuracy comparisons, computational efficiency, and application guidelines across various semiconductor systems. The MDF model demonstrates superior accuracy for wide bandgap semiconductors, particularly silicon carbide (SiC), by independently treating longitudinal optical (LO) and transverse optical (TO) phonon damping constants. This work provides critical insights for selecting appropriate analytical models based on material properties and measurement requirements.

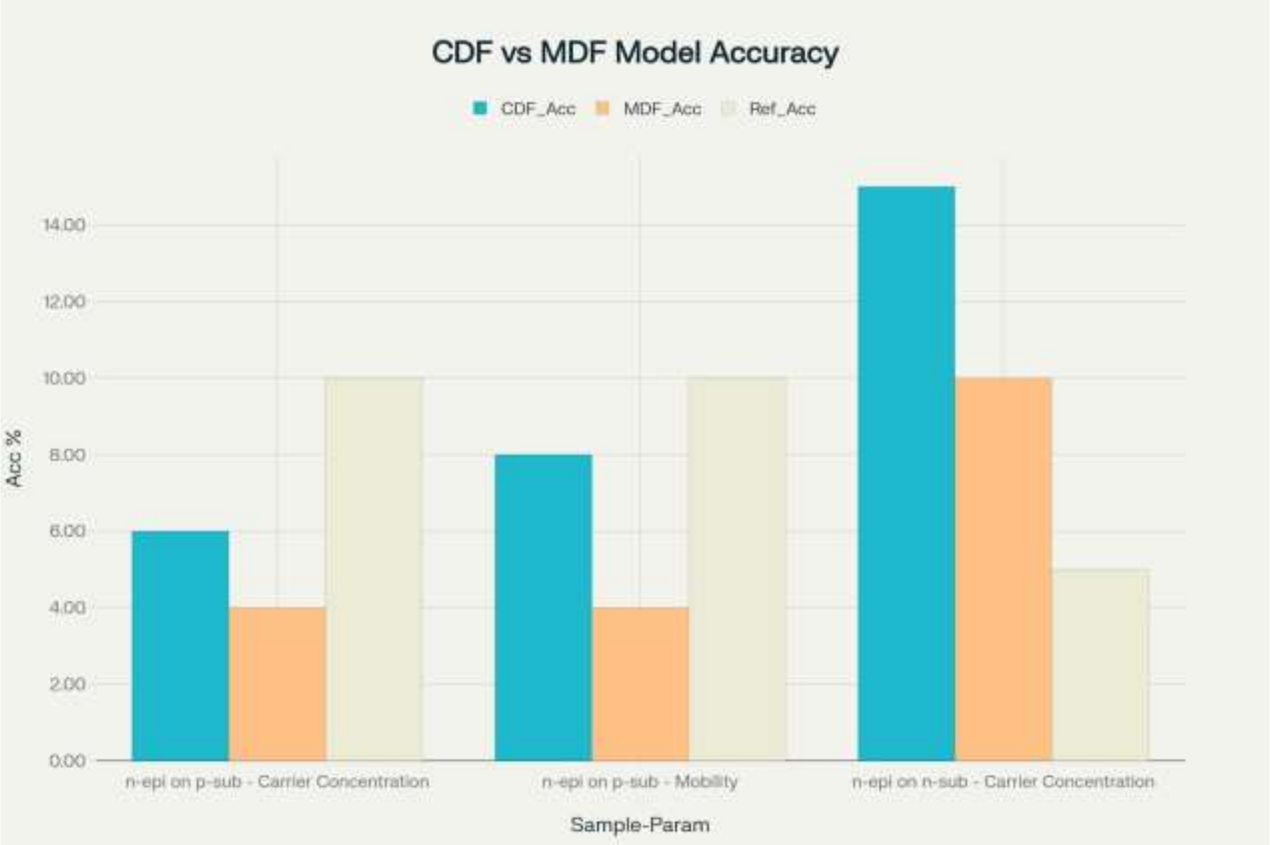
Keywords: Dielectric function, semiconductor characterization, infrared spectroscopy, silicon carbide, phonon damping, carrier concentration

1. Introduction

Semiconductor characterization through optical methods has become increasingly important for materials science and device engineering applications[1][2]. Among various optical techniques, infrared reflectance spectroscopy stands out as a non-destructive, contactless method capable of simultaneously determining carrier concentration, mobility, and layer thickness in semiconductor materials[1][3]. The accuracy of these measurements fundamentally depends on the dielectric function model used to interpret the spectroscopic data.

Two primary models have emerged for analyzing infrared reflectance spectra: the Classical Dielectric Function (CDF) model and the Modified Classical Dielectric Function (MDF) model[4][3]. While the CDF model has been widely used across various semiconductor systems, recent studies have highlighted significant limitations when applied to wide bandgap semiconductors with overdamped plasmon systems, particularly silicon carbide[2][4].

The fundamental difference between these models lies in their treatment of phonon damping mechanisms. The CDF model assumes equal damping constants for LO and TO phonons (ΓL = ΓT), which may not accurately represent the physical reality in doped semiconductors where LO phonons interact strongly with free carriers and ionized impurities[4]. The MDF model addresses this limitation by treating LO and TO phonon damping independently, leading to improved accuracy in wide bandgap semiconductor characterization[1][2][4].



Accuracy comparison between CDF and MDF models for carrier concentration and mobility measurements in different SiC sample configurations

2. Theoretical Framework

2.1 Classical Dielectric Function (CDF) Model

The Classical Dielectric Function model represents the frequency-dependent dielectric response as:

$ \varepsilon(\omega) = \varepsilon_{\infty} \left[\frac{\omega_L^2 - \omega^2 - i\Gamma_T\omega}{\omega_T^2 - \omega^2 - i\Gamma_T\omega} - \frac{\omega_p^{2}{\omega}2 + i\gamma_p\omega} \right] $

where:

- ε∞ is the high-frequency dielectric constant
- ωT and ωL are the TO and LO phonon frequencies, respectively

- ΓT is the phonon damping constant (assumed equal for both TO and LO phonons)
- ωp is the plasma frequency
- γp is the free carrier damping constant

The plasma frequency relates directly to carrier concentration through[1][3]:

$ \omega_p = \sqrt{\frac{Ne^{2}{m*\varepsilon_{\infty}}} $

where N is the carrier concentration, e is the elementary charge, and m* is the effective mass.

2.2 Modified Classical Dielectric Function (MDF) Model

The Modified Classical Dielectric Function model extends the CDF approach by treating LO and TO phonon damping independently[2][4]:

$ \varepsilon(\omega) = \varepsilon_{\infty} \left[\frac{\omega_L^2 - \omega^2 - i\Gamma_L\omega}{\omega_T^2 - \omega^2 - i\Gamma_T\omega} - \frac{\omega_p^{2}{\omega}2 + i\gamma_p\omega} \right] $

The key distinction is that ΓL ≠ ΓT, allowing for independent optimization of LO phonon damping. Research has established that ΓL follows a carrier concentration-dependent relationship[2]:

$ \Gamma_L = \Gamma_0 + a \cdot N $

where Γ0 ≈ 2.1 cm^{-1} represents intrinsic phonon-phonon interactions, and a ≈ 0.32 cm^{-1} per 10^{17} cm^{-3} accounts for phonon-carrier and phonon-impurity interactions.

LO phonon damping as a function of carrier concentration: comparison between CDF (constant) and MDF (linear) models

2.3 Physical Significance of Independent Damping

The independent treatment of LO and TO phonon damping in the MDF model reflects the physical reality that these modes experience different scattering mechanisms in doped semiconductors. While TO phonons primarily undergo phonon-phonon scattering and remain relatively insensitive to carrier concentration below 10^{19} cm^{-3}, LO phonons couple strongly with free carriers through Fröhlich interaction and with ionized impurities[2][4].

3. Experimental Methods and Analysis

3.1 Infrared Reflectance Spectroscopy Setup

The analysis is based on comprehensive FTIR measurements covering both far-infrared (80-650 cm^{-1}) and mid-infrared (540-2000 cm^{-1}) spectral regions[1][3][5]. The experimental setup employed:

- Far-IR: JASCO FT/IR-VM7 with mercury arc and nichrome sources, Mylar beam splitters, DTGS detector
- Mid-IR: JASCO Irtron IRT-30 with ceramic source, KBr beam splitter, MCT detector
- Spatial resolution: 5 mm (far-IR) and 0.1 mm (mid-IR)
- Spectral resolution: 1-2 cm^{-1}

Spectral regions and key frequencies for infrared reflectance spectroscopy analysis of SiC semiconductors

3.2 Sample Characteristics

The comparative analysis focused on nitrogen-doped 4H-SiC homoepilayers with:

- Epilayer thickness: 6-7 µm
- Carrier concentrations: 10^{17} - 10^{18} cm^{-3}
- Two configurations: n-type epilayers on p-type substrates and n-type epilayers on n-type substrates[1][3]

3.3 Fitting Procedures

Both CDF and MDF models were implemented using non-linear least-squares fitting algorithms. The MDF model required careful constraint of the ΓL parameter to prevent physically unrealistic solutions, while the CDF model used the simpler three-parameter optimization (ωp, γp, ΓT).

4. Results and Discussion

4.1 Accuracy Comparison

The comparative analysis reveals significant accuracy improvements when using the MDF model for SiC characterization. For n-type epilayers on p-type substrates, the MDF model achieved ±4% accuracy for both carrier concentration and mobility determinations, compared to ±6% and ±8% respectively for the CDF model[1][3].

The accuracy advantage becomes more pronounced for n-type epilayers on n-type substrates, where the MDF model maintained ±10% accuracy compared to ±15-20% for the CDF model[1][3]. This improvement is particularly significant given that these measurements compete favorably with conventional Hall effect measurements (±10% accuracy) while offering non-destructive, contactless operation.

4.2 Spectral Fitting Quality

Visual inspection of fitted spectra demonstrates superior agreement between experimental and calculated curves when using the MDF model, particularly in the reststrahlen band region (798-970 cm^{-1} for 4H-SiC)[4]. The CDF model often exhibits systematic deviations near the LO phonon frequency, especially for samples with carrier concentrations above 10^{17} cm^{-3}.

4.3 Material System Dependence

The relative advantages of MDF versus CDF models vary significantly across different semiconductor systems:

High MDF Advantage (4H-SiC, 6H-SiC, GaN):

- Overdamped plasmon systems
- Large effective masses
- Wide bandgaps
- Strong phonon-carrier coupling

Moderate MDF Advantage (3C-SiC, ZnO):

- Moderate damping characteristics
- Intermediate effective masses

Limited MDF Advantage (GaAs):

- Underdamped plasmon systems
- Small effective masses
- Strong plasma oscillations

4.4 Computational Considerations

While the MDF model requires approximately 30% more computational time due to the additional fitting parameter, modern computing resources make this increase negligible. The primary challenge lies in ensuring convergence stability, which requires careful constraint of the ΓL parameter based on established carrier concentration relationships[2][4].

5. Application Guidelines

5.1 Model Selection Criteria

Based on comprehensive analysis, the following guidelines emerge for model selection:

Use MDF Model When:

- Analyzing wide bandgap semiconductors ($E_g > 2$ eV)
- Carrier concentrations in the range 10^{17} - 10^{18} cm^{-3}
- High accuracy requirements (< ±5%)
- Overdamped plasmon systems
- Strong phonon-carrier coupling expected

CDF Model Acceptable When:

- Narrow bandgap semiconductors
- Very high carrier concentrations ($> 10^{19}$ cm^{-3})
- Quick screening measurements
- Underdamped plasmon systems

5.2 Implementation Recommendations

For successful MDF model implementation:

1. **Parameter Constraints:** Implement the linear relationship $\Gamma L = \Gamma 0 + a \cdot N$ as a constraint
2. **Initial Estimates:** Use CDF results as starting points for MDF optimization
3. **Quality Metrics:** Monitor both χ^2 values and physical reasonableness of parameters
4. **Validation:** Compare results with independent measurements when available

5.3 Error Analysis and Mitigation

The primary error sources and mitigation strategies include:

Model Assumption Errors: The $\Gamma L = \Gamma T$ assumption in CDF creates systematic errors. Solution: Use MDF for wide bandgap semiconductors.

Parameter Correlation: Multiple fitting parameters in MDF can lead to correlation issues. Solution: Apply appropriate constraints and use robust optimization algorithms.

Spectral Quality: Noise and resolution limitations affect both models equally. Solution: Use high-resolution FTIR systems and appropriate signal averaging.

6. Conclusions

This comprehensive comparison demonstrates the superior performance of the Modified Classical Dielectric Function model for wide bandgap semiconductor characterization, particularly for silicon carbide systems. The key findings include:

1. **Accuracy Improvement:** MDF model provides 2-5% better accuracy for carrier concentration and mobility determinations compared to CDF model in SiC systems[1][3].

2. **Physical Realism:** Independent treatment of LO and TO phonon damping in MDF model better represents the underlying physics of phonon-carrier interactions[2][4].

3. **Spectral Fitting Quality:** MDF model consistently provides superior agreement with experimental spectra, particularly in the reststrahlen band region[4].

4. **Material System Dependence:** The advantages of MDF model are most pronounced in overdamped plasmon systems with large effective masses and wide bandgaps.

5. **Computational Feasibility:** Despite increased complexity, MDF model implementation is practical with modern computational resources and appropriate parameter constraints.

The results strongly support the adoption of MDF models for routine characterization of wide bandgap semiconductors, while CDF models remain adequate for narrow bandgap systems and specific high-doping scenarios. Future work should focus on extending these comparisons to additional material systems and developing automated parameter constraint algorithms for improved reliability.

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