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Solving Strategy for Silicon Carbide Epitaxial Layer Thickness Based on Nonlinear Least Squares Method

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Abstract

Silicon Carbide (SiC) is a pivotal semiconductor material for next-generation high-power and high-frequency electronics, where precise measurement of its epitaxial layer thickness is crucial. This paper presents a robust method for determining this thickness using infrared interference and a nonlinear least squares optimization framework.

We first establish a dual-beam interference model based on the Fresnel equations and Snell's law, deriving reflectivity as a function of thickness and wavelength. The Drude model is incorporated to account for the refractive index dispersion influenced by carrier concentration. For thickness inversion, experimental reflectivity data from SiC wafers is processed by excluding the anomalous "reststrahlen band" (700-1000 cm^{-1}). A hybrid algorithm combining differential evolution for global initial guess generation and nonlinear least squares for local refinement is implemented, yielding a thickness of 7.921 μm with a high goodness-of-fit ($R^2 \approx 0.94$).

Furthermore, we analyze multi-beam interference, deriving its necessary conditions: high interface reflectivity, sufficient coherence length, and layer stability. An adaptive hybrid interference model is developed, dynamically applying dual or multi-beam theory based on local optical conditions. Applied to silicon wafer data, it identifies multi-beam regions and calculates a thickness of 3.765 μm. Re-evaluating the SiC data with this model and a region-weighted strategy to mitigate multi-beam effects in the 399.7-666.3 cm^{-1} band yields an optimized thickness of 7.049 μm. This work provides a reliable and adaptable framework for high-precision thickness characterization in semiconductor engineering.

Keywords

Nonlinear Least Squares Method; Fresnel Equations; Hybrid Interference Model; Drude Model; Differential Evolution

1. Introduction

In recent years, Silicon Carbide (SiC) has garnered significant attention as an emerging semiconductor material. The thickness of the SiC epitaxial layer is a critical parameter influencing material performance, making the establishment of a rapid and accurate measurement method essential. This paper utilizes infrared interference methods to measure epitaxial layer thickness, requiring the development of a mathematical model based on optical mechanisms, exploring its reliability, and designing models to enhance measurement accuracy.

Based on this background, a mathematical model and algorithm are required to address the following problems:

Problem 1: Assuming only single reflection and transmission occur at the epitaxial layer-substrate interface, establish a measurement model for epitaxial layer thickness based on infrared interference. Use Fresnel equations to calculate reflection coefficients for s- and p-polarized components at each interface, derive the total reflectivity expression, and invert the epitaxial layer thickness.

Problem 2: Based on the mathematical model from Problem 1, design a suitable algorithm to determine the epitaxial layer thickness using data from Annexes 1 and 2, and analyze the reliability of the results.

Problem 3: Considering multiple reflections and transmissions within the epitaxial layer leading to multi-beam interference, derive the necessary conditions for multi-beam interference, analyze whether multi-beam interference occurs in data from Annexes 3 and 4, and calculate the silicon epitaxial layer thickness. Using the necessary conditions and model from Problem 3, recalculate the SiC epitaxial layer thickness from Annexes 1 and 2.

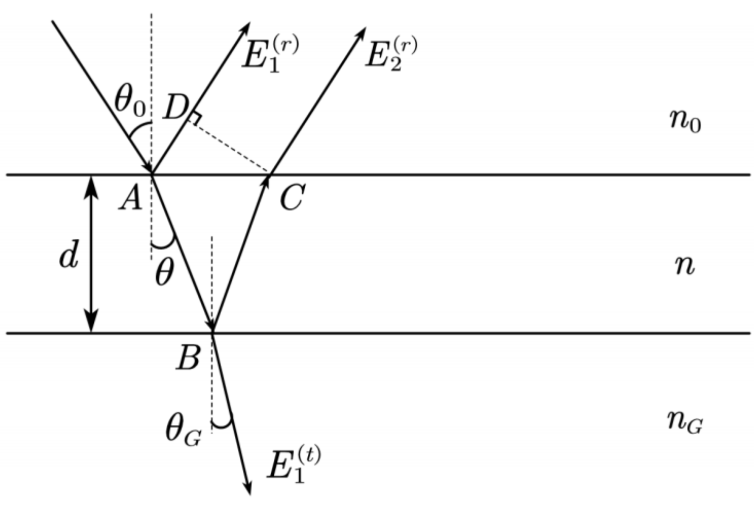

Figure 1. Interference model

2. Model Establishment and Solution

2.1. Dual-Beam Interference Model

For Problem 1, a dual-beam interference model was established. When infrared light is incident on the SiC epitaxial layer, reflections occur at the air-epitaxial and epitaxial-substrate interfaces, producing two coherent beams $E_1$and(E_2. The optical path difference Δdetermines the interference fringe distribution. Using Fresnel equations, reflection coefficients for s- and p-polarized components were calculated, leading to the total reflectivity expression for thickness inversion.

$$\delta = \frac{4\pi nd\cos\theta}{\lambda}$$

where n is the refractive index, d is the thickness, theta is the refraction angle, and lambda is the wavelength.

The reflectivity R for non-polarized light is the average of s- and p-components:

$$R = \frac{R_s + R_p}{2}$$

2.2. Thickness Inversion Algorithm

For Problem 2, data from Annexes 1 and 2 were visualized, identifying anomalous reflection peaks in the$700 - 1000\mathrm{cm}^{-1}$ range due to the reststrahlen band. This region was excluded, and inversion was performed on the $1300 - 4000\mathrm{cm}^{-1}$band. The Drude model was selected for its high goodness-of-fit (R^2 $\approx$ 0.94). A combination of differential evolution (for global search) and nonlinear least squares (for local refinement) was used to invert the thickness, yielding $d = 7.921\mu\mathrm{m}$.

2.3. Multi-Beam Interference Model

For Problem 3, necessary conditions for multi-beam interference were derived:

1. High interface reflectivity: $r_1^2 r_2^2 \geq 0.05$
2. Source coherence length: $L_c \geq 2nd\cos\theta$
3. Stability of thickness and interface roughnes

The multi-beam interference reflectivity is:

$$R = \frac{r_1^2 + r_2^2 + 2r_1 r_2\cos\delta}{1 + r_1^2 r_2^2 + 2r_1 r_2\cos\delta}$$

An adaptive hybrid model was developed to switch between dual- and multi-beam interference based on local reflectivity conditions. For silicon wafers (Annexes 3 and 4), the multi-beam interference region was 399.7 – 635.9cm^{-1}, and the thickness was found to be 3.765 μm. For SiC wafers, the multi-beam region was 399.7 – 666.3 cm^{-1}. A region-weighted strategy was applied, and re-inversion yielded an optimized thickness of 7.049 μm.

3. Conclusions

This study established interference models for SiC epitaxial layer thickness measurement. The nonlinear least squares method, combined with differential evolution, effectively solved the inversion problem. The adaptive hybrid interference model and region-weighted strategy improved accuracy by addressing multi-beam interference and material-specific anomalies. The proposed methods are reliable and applicable to semiconductor material characterization in advanced engineering contexts.

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