Determination of Silicon Carbide Epitaxial Layer Thickness Based on Genetic Algorithm and Transfer Matrix Model

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Abstract. This paper focuses on determining the thickness of silicon carbide epitaxial layers using infrared interferometry. A mathematical model was established based on the principle of double-beam interference, incorporating Snell’s Law and the Pythagorean theorem to calculate the optical path difference between two reflected beams (from the epitaxial layer surface and the substrate interface). The phase difference was linked to the interference order, and conditions for constructive and destructive interference were analyzed to derive the fundamental thickness model. The Sellmeier dispersion model was introduced to account for the wavelength-dependent refractive index influenced by doping concentration. For experimental verification, the reflectance spectra were preprocessed to remove noise and convert wavenumbers into wavelengths. Extreme interference points were identified, and thickness was optimized globally using genetic algorithms in MATLAB, minimizing the least-squares error between modeled and measured reflectance. Reliability was confirmed through residual analysis and consistency across incidence angles. The impact of multi-beam interference was analyzed by comparing its characteristics with double-beam interference and identifying necessary conditions (e.g., high reflectivity and phase stability). The coefficient of variation in wavenumber spacing was used to multi-beam effects. For silicon wafers, the transfer matrix model and genetic algorithms were employed to calculate optimized thickness, accounting for multi-beam interference. This work provides a robust framework for high-accuracy, nondestructive thickness measurement of epitaxial layers.

Keywords: Genetic Algorithm, Transfer Matrix Model (Tmm), Sellmeier Equation, Spectral Data Inversion.

1. Introduction

As an emerging third-generation semiconductor material, silicon carbide has been gaining increasing attention in related fields due to its superior comprehensive performance [1][2]. As a key parameter of epitaxial materials, the thickness of silicon carbide epitaxial layer has a direct impact on device performance [3]. Therefore, it is urgent and important to formulate a scientific, accurate and reliable test standard for the thickness of silicon carbide epitaxial layer. The epitaxial layer is a single crystal thin film formed on a single crystal substrate by epitaxial growth technology. Its thickness is one of the core indicators for judging the performance of semiconductor devices [4]. Infrared interferometry is the mainstream non-destructive method for measuring the thickness of epitaxial layer. Its core working principle is: the epitaxial layer and the substrate have different refractive indices due to the difference in doping carrier concentration. When infrared light is incident on the epitaxial layer, part of the light is reflected from the surface of the epitaxial layer (reflected light 1), and the other part of the light penetrates the epitaxial layer and is reflected from the surface of the substrate (reflected light 2). The two beams of reflected light will produce interference fringes under certain conditions. The thickness of the epitaxial layer can be determined by parameters such as the wavelength of the infrared spectrum, the refractive index of the epitaxial layer and the incident angle of the infrared light [5-10]. It should be noted that the refractive index of the epitaxial layer is not a constant value. Its size is closely related to parameters such as the doping carrier concentration and the wavelength of the infrared spectrum. This characteristic will have a direct impact on the accuracy of thickness measurement.

Based on existing research, this paper focuses on the application of infrared interferometry to measure the thickness of silicon carbide and silicon epitaxial layers. Taking into account the nonconstant nature of the epitaxial layer's refractive index and different interference phenomena, we conduct research in different scenarios:

First, under the assumption that only a single reflection and transmission at the epitaxial layer-substrate interface is considered, and incorporating the working principles of infrared interferometry, a mathematical model for determining epitaxial layer thickness is established.

Second, based on the previously established mathematical model, an algorithm for determining epitaxial layer thickness is designed. Furthermore, measured spectral data (including wavenumbers and interference spectral reflectance) from the same silicon carbide wafer is substituted into the algorithm to calculate thickness, and the reliability of the calculated results is analyzed.

Finally, we further consider the scenario of multiple reflections and transmissions of light waves at the epitaxial layer-substrate interface. We first derive the necessary conditions for generating multi-beam interference and the potential impact of this interference pattern on the accuracy of epitaxial layer thickness calculations. Secondly, combined with the test data of the same silicon wafer (the data includes wavenumber and interference spectrum reflectivity), determine whether multi-beam interference occurs in the test results of the silicon wafer, and based on this, provide a mathematical model and algorithm for determining the thickness of the silicon epitaxial layer, and finally obtain the thickness calculation result; in addition, it is also necessary to determine whether multi-beam interference also exists in the test results of the silicon carbide wafers in Attachments 1 and 2. If this interference phenomenon affects the calculation accuracy of the silicon carbide epitaxial layer thickness, it is necessary to optimize the model to eliminate its influence, and provide the thickness calculation result after eliminating the influence.

2. Problem Analysis and Model Assumptions

2.1. Problem Analysis

In analyzing single reflections and transmissions at the epitaxial layer-substrate interface, the interference phenomena arising from these single interactions are of primary interest, allowing the cumulative loss in light intensity to be neglected. This problem is addressed through an integrated approach combining mathematical geometric analysis with physical optical models.

The core of thickness measurement via interference lies in the accurate determination of the optical path difference (OPD). Key factors influencing OPD must be carefully considered. Firstly, half-wave loss requires attention: as light propagates from air (optically rarer medium) into the epitaxial layer (optically denser medium) and then into the substrate (optically rarer medium), a π phase shift occurs upon reflection at the "low-to-high refractive index" interface. This phase alteration must be incorporated into the OPD calculation. Secondly, the refractive index is not constant but varies with parameters such as dopant carrier concentration and the wavelength of the infrared spectrum. Thus, it necessitates determination through physical models like dispersion relations (e.g., Cauchy model) or local polynomial fitting. The OPD can be computed using Snell's Law (to determine the refraction angle) and geometric path analysis (e.g., the Pythagorean theorem).

Furthermore, interference conditions must be defined. Constructive interference (bright fringes) requires the OPD to be an integer multiple of the wavelength ($\Delta = m\lambda$, $m \in Z$), while destructive interference (dark fringes) occurs when the OPD is a half-integer multiple of the wavelength ($\Delta = (m + 1/2)\lambda$). Combining the OPD expression with these interference conditions allows for the derivation of a quantitative model relating thickness to interference fringes. Consistent units must be maintained throughout calculations.

Based on the thickness model derived, experimental data (e.g., wavenumber-reflectivity pairs from appendices) can be used for numerical computation. This involves converting wavenumbers to wavelengths and generating reflectance spectra using MATLAB (note unit consistency). Subsequent peak and valley detection algorithms (amplitude or derivative-based) identify adjacent extremum points in the reflectance spectrum. Thickness can be calculated using two primary methods: an analytical approach based on the wavenumber difference between adjacent extrema (e.g., d =

1/(2nΔνcosθ)), or by performing nonlinear least-squares fitting of the entire theoretical reflectance model to the experimental data. To obtain the optimal thickness estimate, optimization algorithms (e.g., genetic algorithms) can be employed to minimize the fitting error or ensure consistency across measurements from different incident angles.

The reliability of the model and algorithm is evaluated using statistical metrics like the coefficient of variation (CV): generally, a smaller CV indicates lower dispersion in thickness estimates and higher result reliability. Regarding multi-beam interference, its impact is assessed by analyzing its characteristics and comparing it with dual-beam interference (e.g., using the Airy formula or transfer matrix models to describe sharper fringes and harmonics). Conditions conducive to multi-beam interference (e.g., higher interface reflectivity, lower layer absorption, good source coherence) are identified through literature review. If multi-beam effects are significant (e.g., the CV of wavenumber intervals exceeds a critical threshold, or dual-beam model residuals show systematic bias), a multi-beam interference model (e.g., Airy formula) should be adopted for recalibration. Ultimately, optimization algorithms and transfer matrix models implemented on platforms like MATLAB can be used for high-precision thickness retrieval.

2.2. Model Assumptions

Based on the above analysis, this paper makes the following assumptions:

① The infrared light source used in the experiment is quasi-monochromatic with good monochromaticity, and the intensity of the light source remains stable.

② The incident angle measurement accuracy meets the experimental requirements, and the incident beam is parallel and does not diverge or converge.

③ The epitaxial layer surface and the interface between the epitaxial layer and the substrate remain flat. Reflected light 1 and 2 in Figure 1 are parallel and coherent, and the test environment is stable.

④ The SiC epitaxial layer and substrate dielectrics remain uniform and isotropic, meaning that the carrier concentration within the same dielectric remains constant. Only the effect of infrared spectrum wavelength on the refractive index of the epitaxial layer is considered.

⑤ The effects of light absorption on the intensity and phase of the reflected light are ignored.

6 The test environment maintains suitable temperature and humidity, is free of external interference light, and the material properties are not affected by external conditions.

3. Modeling and solving

Since the doping carrier concentration is affected by the doping process, material properties, etc. [10], the doping carrier concentration of SiC for different applications varies and is quite specific. To ensure the universality of the model, this paper assumes that SiC has a low doping carrier concentration, that is, ignores its effect on the refractive index, and chooses the Sellmeier equation to describe the effect of infrared spectrum wavelength on the refractive index [8].

The Sellmeier equation is mainly used to describe the dispersion phenomenon of the refractive index of a transparent medium as it changes with the wavelength of the incident light. It is widely used in lens design, optical fiber communication, calculation of phase matching conditions for laser crystals, thin film detection, and other fields [8]. Its standard form is as follows:

$$n^2(\lambda) = 1 + \sum_i \frac{B_i \lambda^2}{\lambda^2 - C_i} \tag{1}$$

The reflectivity of SiC is expressed as:

$$n^2(\lambda_i) = 1 + \frac{a{\lambda_i}^2}{{\lambda_i}^2 - A} + \frac{b{\lambda_i}^2}{{\lambda_i}^2 - B} + \frac{c{\lambda_i}^2}{{\lambda_i}^2 - C} \tag{2}$$

Where a,b,c represents the oscillator strength, which are both material constants; A, B,C represents the corresponding infrared spectrum wavelength. Based on the experimental data, paying attention to unit conversion, we can use MATLAB to generate two reflection spectra for incident angles of and , and find the maximum and minimum values. Reflectance spectroscopy can identify chemical and physical characteristics. Since the two spectra are measured on the same silicon carbide wafer, they should be nearly identical. Overlaying the two spectra confirmed their near-identical alignment, verifying their accuracy. Combined with the reflectance spectrum, the extreme points and corresponding data can be obtained as shown in Table 1 and Table 2:

Table 1. Extreme data (The incident angle is $10°$)

	Wavelength/μm	**Reflectivity**		**Wavelength/μm**	**Reflectivity**
Minimum	433.00	0.22	Maximum	520.00	0.34
	575.00	0.28		636.00	0.36
	661.00	0.34		828.00	0.95
	1001.00	0.03		1012.00	0.04
	1036.00	0.01		1084.00	0.09
	1128.00	0.07		1213.00	0.13
	1276.00	0.11		1396.00	0.15
	1475.00	0.14		1543.00	0.16
	1551.00	0.16		1598.00	0.17
	1712.00	0.15		1835.00	0.18
	1949.00	0.16		2078.00	0.18
	2199.00	0.17		2321.00	0.18

According to the thickness measurement model and the extreme point data mentioned above, the genetic algorithm can be used to obtain the thickness of multiple epitaxial layers containing parameters. The incident angles are different, but the same SiC wafer is being tested, and the parameters should be fixed values. Therefore, the next step is to use MATLAB programming to screen and measure the parameters using the genetic algorithm. The fitness value is used to determine whether the parameters are the optimal solution. The parameter group corresponding to the maximum fitness value can determine the relationship between the refractive index and the wavelength. In the actual calculation process, it was found that when solving the conditional formula of the refractive index, using two sets of parameters is more realistic than using three sets of parameters, and the model accuracy is higher. Therefore, formula (1) is optimized to formula (3), that is:

$$n^2(\lambda_i) = 1 + \frac{a\lambda_i^2}{\lambda_i^2 - A} + \frac{b\lambda_i^2}{\lambda_i^2 - B} \tag{3}$$

According to the genetic algorithm, the average thickness is 10.198.

This paper uses the coefficient of variation of thickness to test reliability. In this case, the coefficient of variation of d is:

$$CV = \frac{\sigma_d}{\mu_d} \tag{4}$$

Table 2. Extreme data (The incident angle is $10°$)

	Wavelength/μm	**Reflectivity**		**Wavelength/μm**	**Reflectivity**
Minimum	438	0.2379	Maximum	521	0.3683
	579	0.3086		639	0.3899
	662	0.3776		703	0.4334
	707	0.4332		918	0.9998
	1003	0.0336		1016	0.0511
	1040	0.0121		1091	0.1058
	1137	0.0735		1222	0.1429
	1288	0.1235		1409	0.164
	1486	0.148		1546	0.1603
	1553	0.1602		1608	0.1741
	1627	0.1731		1636	0.1734
	1731	0.1598		1862	0.1832
	1968	0.1681		2099	0.1873
	2216	0.1736		2321	0.1839
	2329	0.1837		2345	0.1847
	2352	0.1847		2366	0.1851
	2368	0.1851		2390	0.1866

Substituting this into the equation, we get $CV = 19.96\%$. It is generally considered that when the CV is less than 20%, the result is reliable. In this case, the coefficient of variation meets the requirements, and the answer is accurate and reliable.

For the thickness measurement scenario under multi-beam interference conditions, this paper uses the transfer matrix method (TMM) combined with the genetic algorithm to determine the thickness. The transfer matrix method decomposes the entire optical structure into interface effects and propagation effects, and uses matrix multiplication to include infinite reflections and transmissions in the reflectivity formula. According to the transfer matrix method (TMM), MATLAB programming is used to solve it. First, formula (2) is combined with TMM to obtain the theoretical reflectivity. Referring to the actual reflectivity in the appendix and combined with the genetic algorithm, the optimal parameters of the refractive index and the thickness of the semiconductor epitaxial layer are obtained through data at two different incident angles. By using the transfer matrix method model, the impact of interference in different situations on the thickness calculation accuracy can be effectively reduced, that is, the model is replaced and the model obtained in Problem 1 is optimized. According to national standards, the refractive index of the substrate is 2.55. At this time, the thickness of the silicon carbide wafer can be calculated as $5.014 \mu m$.

4. Conclusions

This paper established a robust framework for determining silicon carbide epitaxial layer thickness by integrating the transfer matrix model (TMM) with genetic algorithm (GA) optimization. The approach effectively combines physical principles with computational intelligence to achieve accurate thickness inversion from infrared reflectance spectra, while accounting for wavelength-dependent refractive index through the Sellmeier equation.

The model demonstrates notable strengths in its theoretical rigor, practical applicability to real-world conditions, generalizability to other semiconductor materials, and computational efficiency. However, limitations persist regarding its dependence on accurate material parameters, computational complexity in large-scale applications, and simplifying assumptions about ideal environmental conditions.

Future research should focus on developing adaptive algorithms to correct parameter deviations, implementing computational optimizations to enhance efficiency, and extending the model to incorporate environmental variables and material imperfections. These improvements would facilitate real-time industrial applications and further strengthen the model's practical utility in semiconductor manufacturing and quality control.

In summary, this work provides an effective methodology for non-destructive thickness measurement with significant potential for both research and industrial applications.

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