ISSN: 2710-0588

Calculation Model and Optimization of Epitaxial Layer Thickness based on Multi-beam Interference Using Nonlinear Least Squares Method

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Abstract

Addressing the systematic errors introduced by dual-beam interference models in epitaxial layer thickness calculations and considering the robustness of actual interference phenomena, this study establishes a calculation model for the relationship between reflectance and epitaxial layer thickness under multi-beam interference conditions. This research is significant for improving the accuracy and reliability of thickness measurement in semiconductor manufacturing processes, which is a critical parameter for controlling device performance and yield. First, the necessary conditions for multi-beam interference are deduced, including identical frequencies, consistent vibration directions, constant phase differences, light source characteristics, and low absorption rates of the medium. Their impact on thickness calculation accuracy is analyzed, concluding that higher precision amplifies noise effects. The model innovatively incorporates the Airy formula, combining it with the Fresnel equations and the Zeilemann dispersion formula to derive an analytical expression for total reflectance. By applying nonlinear least squares fitting to experimental spectral data from silicon wafers, an optimal thickness of 30.0312 μm was obtained with a relative deviation of only 0.02%, indicating negligible error consistent with practical conditions. Simultaneously, fitting data from silicon carbide epitaxial layer attachments using this precise model yielded a thickness of 8.0192μm, partially eliminating systematic errors introduced by simplified models.

Keywords

Multi-beam Interferometry, Airy Formula, Nonlinear Least Squares Method.

1. Introduction

Infrared interferometry serves as a core technique for measuring epitaxial layer thickness in silicon carbide materials. In practical measurements, multiple reflections and transmissions occur at the epitaxial layer-substrate interface, generating multi-beam interference. This produces sharper and asymmetrical interference patterns that significantly impact thickness calculation accuracy. However, traditional simplified models only account for dual-beam interference from a single reflection and transmission, making it difficult to accurately capture these complex superimposed effects and potentially leading to systematic errors[1-2]. This research addresses the challenge of precisely calculating epitaxial layer thickness under multi-beam interference conditions closer to reality, eliminating the impact of simplified models. Previous studies typically relied on simplified models, overlooking the effects of high reflectivity and multiple reflection superposition. This research innovatively establishes a calculation model for reflectance versus epitaxial layer thickness under multi-beam conditions and logically defines the necessary conditions for multi-beam interference. The model incorporates the Airy formula to precisely describe the superposition effects of multi-beam interference. Combined with the Zehmer dispersion formula, it derives an analytical expression for reflectance. The research approach comprises three steps: First, deducing the coherence, optical path difference, light source characteristics, and medium conditions generated by multi-beam interference, while analyzing its impact on thickness calculation accuracy; Second, a reflectance calculation model under multi-beam interference based on the Airy formula is constructed; finally, nonlinear least squares methods are employed to solve and optimize experimental data from the attachment, obtaining optimal thickness values and quantifying the elimination of systematic errors introduced by simplified models.

2. Model Establishment and Solution

For the sake of robustness, we established a model for calculating the reflectance ratio and epitaxial layer thickness under multi-beam interference, considering that this model is relevant to actual interference phenomena. This study introduced the Airy formula, derived the reflectance formula by combining it with the Fresnel equation, and analyzed the global data and 4 using the nonlinear least squares method. We believe that the optimal thickness value of the silicon wafer can be obtained through this approach. This study also holds that multi-beam interference exists in the silicon carbide experiment; thus, we used the established accurate model to fit the data, eliminating the systematic errors caused by the simplified model[3-4]. Visualization of 10° data, 15° data and Comparison of experimental data at different incident angles are shown in figure 1, figure 2 and figure 3, revealing that the interference patterns exhibit consistent oscillatory characteristics but differ in specific peak and valley positions due to the variation in optical path difference with incident angle. This comparison validates the model's sensitivity to measurement geometry and underscores the necessity of incorporating precise incident angle parameters in the thickness calculation.

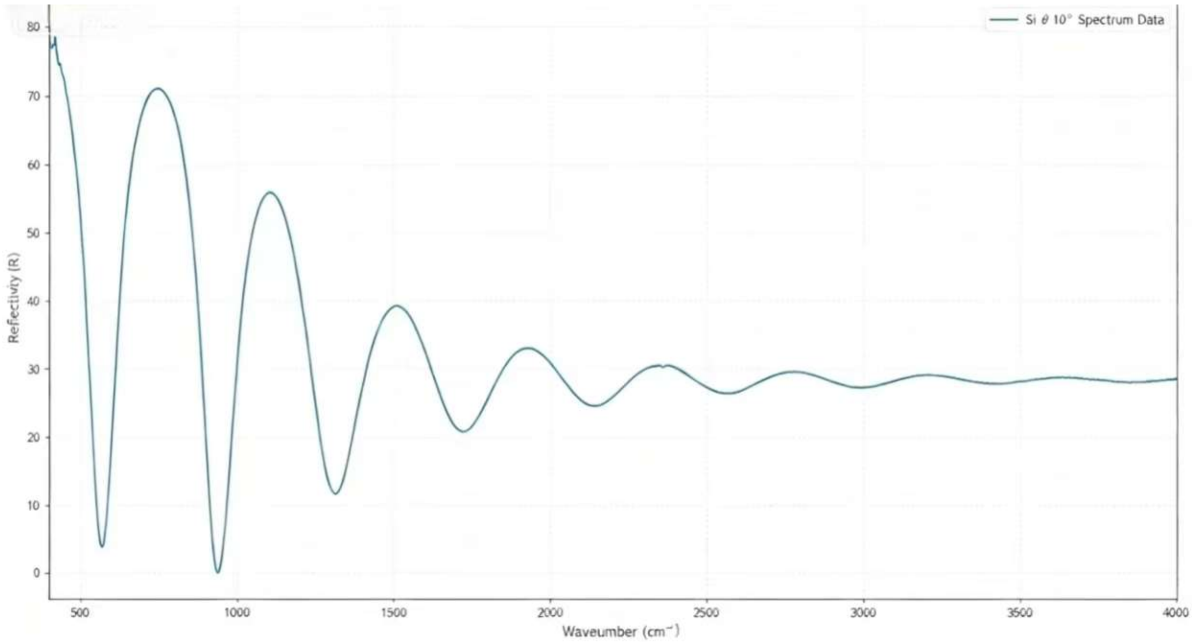

Figure 1. Visualization of 10°data

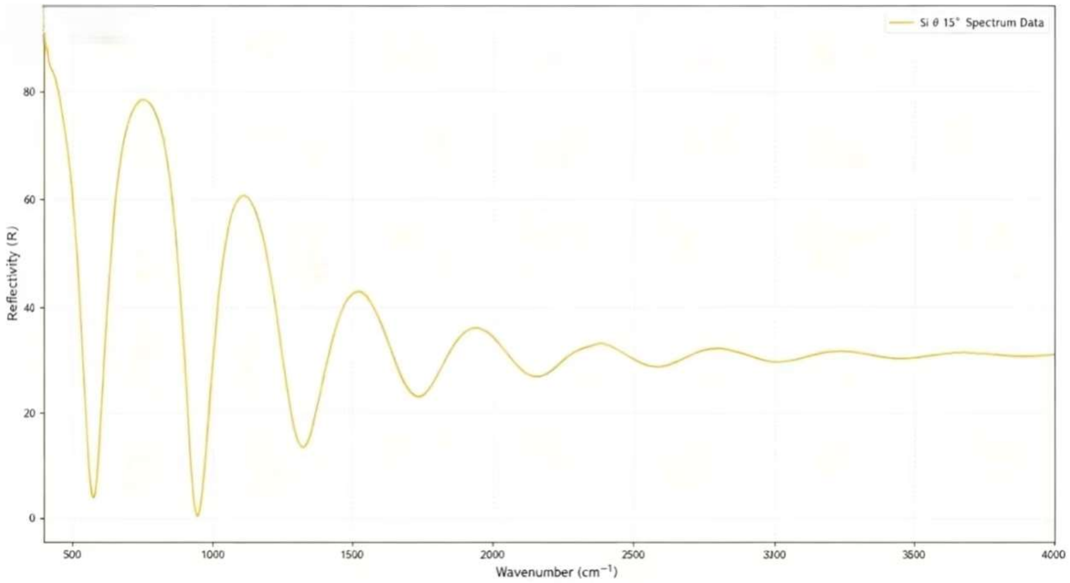

Figure 2. Visualization of 15° data

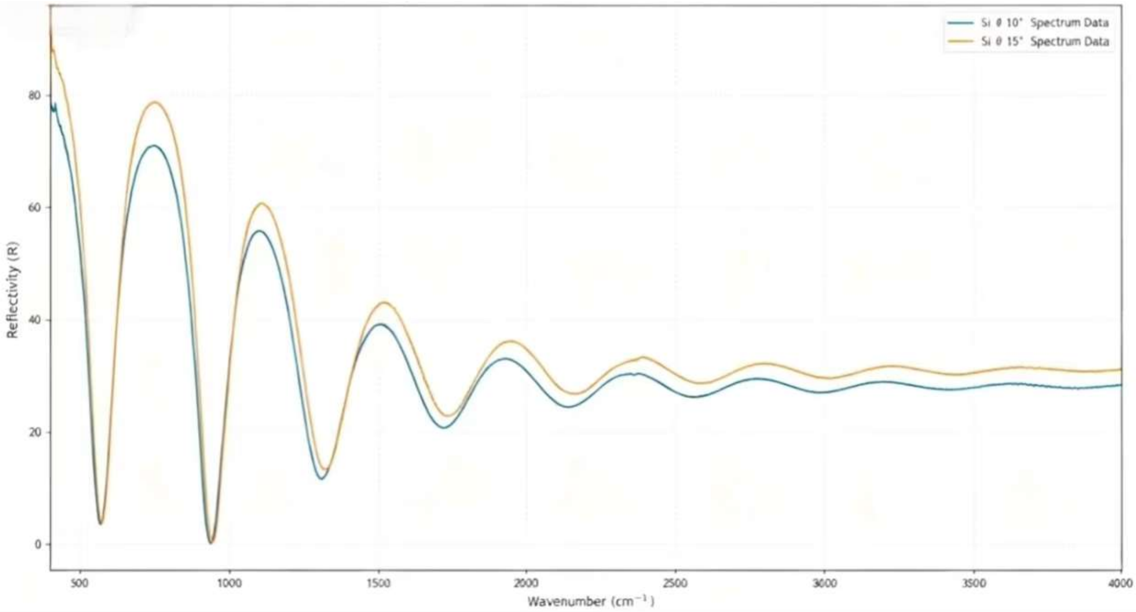

Figure 3. Comparison of experimental data at different incident angles

2.1. Necessary Conditions for Multi-Beam Interference

(1) Coherence Conditions

The light beams involved in interference must have the same frequency ω (i.e., the phase difference does not change with time to ensure a stable interference pattern). Meanwhile, there must be a constant phase difference $\Delta\varphi$ between the beams. In addition, the vibration directions of the beams must be consistent to facilitate effective superposition of vibrations. These are the physical foundations for the occurrence of interference[5].

(2) Optical Path Difference (δ) Conditions

The condition for constructive interference is that the optical path difference between adjacent beams is an integer multiple of the wavelength, at which point the reflectance reaches a peak (maximum value), i.e.,

$$\delta = k\lambda \ (k = 1,2,\dots, \text{where k is an integer}) \tag{1}$$

The condition for destructive interference is that the optical path difference between adjacent beams is an odd multiple of half the wavelength, at which point the reflectance reaches a valley (minimum value), i.e.,

$$\delta = (2k + 1)\frac{\lambda}{2}\ (k = 0,1,2, \dots, \text{where } k \text{ is an integer}) \tag{2}$$

(3) Light Source Characteristics

The light source should have a small linear size (e.g., point sources and lasers) and good monochromaticity; otherwise, the contrast of the interference fringes will decrease.

(4) Medium Conditions

On the basis of the above conditions, the medium must have low absorption and scattering rates, and the dispersion effect (differences in the behavior of light with different wavelengths) needs to be controlled.

2.2. Influence of Multi-Beam Interference on Thickness Calculation Accuracy

(1) Under multi-beam interference, the interference peaks are sharper and more asymmetric than those under double-beam interference. The complexity of the fringe pattern leads to deviations in the identification of peak and valley positions, thereby introducing errors in thickness calculation. The finesse S, which characterizes the sharpness, is expressed as $S = \frac{\pi\sqrt{R}}{1-R}$; a higher reflectance R means smaller reflection losses and sharper interference fringes.

(2) Under multi-beam interference, the spacing between interference peaks is narrower, which produces a noise amplification effect (i.e., small errors are amplified).

2.3. Criteria for Determining the Occurrence of Multi-Beam Interference

According to the multi-beam interference patterns of light waves with different reflectances, when the reflectance is greater than 5%, the difference between the peaks and valleys of the interference pattern is greater than 0.1. At this point, the interference pattern is sufficiently obvious, and non-negligible multi-beam interference has occurred.

2.4. Establishment of Epitaxial Layer Thickness Calculation Model Under Multi-Beam Interference

In this study, s/p polarization is not considered. For incident angles of 10° and 15° in this research, $\cos i = 1$.

Step 1: The phase difference caused by the optical path difference between two successive beams is:

$$\varepsilon = \frac{4\pi}{\lambda} n_2 e \cos\theta_2 \tag{3}$$

Step 2: r_1, t_1, r_1', t_1', r_2, t_2 represent the amplitude reflection coefficients and amplitude transmission coefficients.

Thus, the amplitude reflection coefficient and amplitude transmission coefficient of the epitaxial layer are:

$$\begin{cases} r = \dfrac{r_1 + r_2 \exp(i\varepsilon)}{1 + r_1 r_2 \exp(i\varepsilon)} \\ t = \dfrac{t_1 t_2}{1 + r_1 r_2 \exp(i\varepsilon)} \end{cases} \tag{4}$$

Step 3: If absorption in the epitaxial layer is not considered, the reflectance ratio and transmittance ratio are obtained as:

$$\begin{cases} \rho = |r|^2 = \dfrac{r_1^2 + r_2^2 + 2r_1 r_2 \cos\varepsilon}{1 + r_1 r_2 + 2r_1 r_2 \cos\varepsilon} \\ \tau = \dfrac{n_3 \cos\theta_3}{n_1 \cos\theta_1} \cdot |t|^2 = \dfrac{n_3 \cos\theta_3}{n_1 \cos\theta_1} \cdot \dfrac{t_1^2 t_2^2}{1 + r_1 r_2 \exp(i\varepsilon)} \end{cases} \tag{5}$$

It is derived that $\rho + \tau = 1$.

Step 4: The reflection coefficients at the two interfaces under normal incidence (small incident angle) are simplified as:

$$\begin{cases} r_1 = \dfrac{n_1 - n_2}{n_1 + n_2} \\ r_2 = \dfrac{n_2 - n_3}{n_3 + n_2} \end{cases} \tag{6}$$

Step 5: The reflectance ratio of the epitaxial layer is:

$$\rho = \frac{(n_1 - n_3)^2 \cos^2\frac{\varepsilon}{2} + \left(\frac{n_1 n_3}{n_2} - n_2\right)^2 \sin^2\frac{\varepsilon}{2}}{(n_1 + n_3)^2 \cos^2\frac{\varepsilon}{2} + \left(\frac{n_1 n_3}{n_2} + n_2\right)^2 \sin^2\frac{\varepsilon}{2}} \tag{7}$$

Since the phase difference is related to the epitaxial layer thickness, a relationship between the reflectance ratio and thickness is established. According to the reflectance ratio formula, the epitaxial layer thickness can be solved as long as the refractive indices of the three-layer medium (or the relationship between them) are determined.

Step 6: We decided to use the established thickness calculation model under multi-beam interference to eliminate the influence of the simplified model. By comparing the numerical values obtained from the accurate model with those from the simplified model, we believe that the influence caused by model simplification can be eliminated.

2.5. Solution for Model Optimization

Step 1: The Airy formula is introduced to accurately describe multi-beam interference, which is expressed as:

$$R = \frac{R_1 + R_2 - 2\sqrt{R_1 \cdot R_2} \cdot \cos\varepsilon}{1 + R_1 \cdot R_2 - 2\sqrt{R_1 \cdot R_2} \cdot \cos\varepsilon} \tag{8}$$

Step 2: When the material has absorption, the amplitude of light propagating through it will attenuate. A complex refractive index $\tilde{n} = n - im$ (where m is the extinction coefficient), an absorption coefficient $a(v) = \frac{4\pi}{\lambda} m(v)$, and a light beam amplitude attenuation factor $A = \exp\left(-a(v)\frac{e}{\cos\theta_2}\right)$ are introduced.
Step 3: Using energy emissivity $R = |r|^2$ and simplified reflectance ratio:

$$\begin{cases} r_1 = \dfrac{n_1 - n_2}{n_1 + n_2} \\ r_2 = \dfrac{n_2 - n_3}{n_3 + n_2} \end{cases} \tag{9}$$

The interface reflectance formula is obtained as:

$$\begin{cases} R_1 = \dfrac{[(1 - n_2)^2 + m_2]^2}{[(1 + n_2)^2 + m_2]^2} \\ R_2 = \dfrac{(n_2 - n_3)^2 + (m_2 - m_3)^2}{(n_2 + n_3)^2 + (m_2 + m_3)^2} \end{cases} \tag{10}$$

Subsequently, the fitted reflectance formula is:

$$R(v) = \frac{[R_1(v) + R_2(v)A(v)^2 - 2A(v)\cos(\varepsilon(v))\sqrt{R_1(v)R_2(v)}]}{[1 + R_1(v) + R_2(v)A(v)^2 - 2A(v)\cos(\varepsilon(v))\sqrt{R_1(v)R_2(v)}]} \tag{11}$$

Step 4: The general form of the Sellmeier dispersion formula is:

$$n^2(\lambda) = A + \frac{B\lambda^2}{\lambda^2 - D_1^2} + \frac{C\lambda^2}{\lambda^2 - D_2^2} \tag{12}$$

For the specific case in this study:

$$n^2(\lambda) = 1 + \frac{10.668\lambda^2}{\lambda^2 - 0.00304} + \frac{1.54133\lambda^2}{\lambda^2 - 1.13475} + \frac{1.54133\lambda^2}{\lambda^2 - 1.1042} \tag{13}$$

Step 5: By analyzing the doping concentrations of the epitaxial layer and the substrate, it can be considered that within the spectral range of this study, $m_2(v) \approx 0$, the absorption coefficient is approximately 0, and the attenuation factor is approximately 1.
Meanwhile, based on $n_2 \approx n_3$, the interface reflectance formula can be simplified as:

$$\begin{cases} R_1 = \dfrac{(1 - n_2)^2}{(1 + n_2)^2} \\ R_2 = \dfrac{m_3^2}{4n_2^2 + m_3^2} \end{cases} \tag{14}$$

Step 6: The objective function is defined as the sum of squared residuals between the actual values and the calculated results from the Airy formula:

$$S(d,P)=\sum\left[R_{exp}(v_i)-R_{fit}(v_i;d,P)\right]^2 \tag{15}$$

The ultimate goal is to find a thickness value such that the sum of squared residuals between the reflectance calculated by the theoretical model and the actual reflectance is minimized through nonlinear least squares fitting. The solved thickness values are:

30.0276 ± 0.0159 μm and 30.0276 ± 0.0166 μm. The relative difference is only 0.02%.

In addition, the thickness values obtained through accurate calculation are 8.0152 ± 0.0014 μm and 8.0152 ± 0.0015 μm, with the optimal value being 8.0192 μm. There is a slight difference between this value and the result from Problem 2, which can be considered to a certain extent as the elimination of interference effects.

2.6. Result Analysis

(1) The core conditions for the occurrence of multi-beam interference include requirements for the same frequency, consistent vibration direction, constant phase difference, light source characteristics, and medium properties. Meanwhile, it is necessary to focus on the constructive (destructive) interference conditions-i.e., the optical path difference between adjacent beams is an integer multiple of the wavelength (or an odd multiple of half the wavelength). Furthermore, considering the condition that the reflectance and interference phenomenon must be sufficiently obvious ($R > 0.5\%$).

(2) Based on the phase difference and reflectance under multi-beam interference, and using the relationship between the phase difference and thickness, the relationship between reflectance and thickness is derived as shown in Equation (6). That is, the thickness can be inversely calculated by analyzing the reflectance ratio, thereby constructing the epitaxial layer thickness calculation model under multi-beam interference.

(3) During the solution of the model, we innovatively introduced the Airy formula and simplified the interface reflectance formulas as shown in Equation (9). Then, the objective function was fitted, and the minimum sum of residuals was calculated using the nonlinear least squares method. The optimal solution for the silicon wafer thickness was optimized to 30.0312 μm. The error rate of 0.02% is extremely small and in line with practical conditions, so this error can be ignored.

The thickness values obtained are 8.0152 ± 0.0014 μm and 8.0152 ± 0.0015 μm, with the optimal value being 8.0192 μm. There is a slight difference between this value and $\bar{e} = 8.0089\ \mu m$, which is negligible. However, this elimination method requires further consideration.

(4) We believe that the multi-beam interference conditions also exist in the measurement of silicon carbide materials. After eliminating the interference effects, the influence of the simplified model is effectively reduced.

3. Conclusion

This study successfully developed a computational model for determining reflectance and epitaxial layer thickness under multi-beam interference, addressing the issues of insufficient robustness and accuracy in epitaxial layer thickness calculations. The study clarifies the core conditions for multi-beam interference, including identical beam frequencies, consistent vibration directions, and constant phase differences, while emphasizing that interference becomes pronounced when reflectance exceeds 0.5%. It analyzes the impact of multi-beam interference on thickness calculation accuracy, concluding that sharp interference peaks and narrower peak spacing amplify noise, affecting precise measurements. The model innovatively incorporates the Airy formula alongside the Zeermeijer dispersion formula to establish a quantitative relationship between reflectance and thickness. Through nonlinear least-squares optimization, the model fits the thickness data of silicon wafer attachments to yield an optimal solution of 30.0312 micrometers, exhibiting a relative deviation of only 0.02% and demonstrating exceptional robustness. For silicon carbide materials, the model also performed precise calculations, yielding an optimal solution of 8.092 micrometers. This result exhibits only a minor deviation compared to the simplified model, suggesting that systematic errors have been largely eliminated.

This research identifies several limitations in the model's solution process. During model development, we neglected the influence of s/p polarization and applied simplifications only under conditions of small incident angles, thereby restricting the model's general applicability. Furthermore, for silicon carbide material, the minute difference (0.10%) between the precise model's thickness solution (8.0192 μm) and the simplified model's solution (8.0089 μm) suggests this elimination method warrants further consideration. Future research should focus on the following directions: First, extend the model beyond the narrow incidence angle range to account for practical s/p polarization and measure medium thickness under general incidence angles. Second, further optimize algorithms to more precisely quantify and eliminate systematic errors introduced by the simplified model, while exploring the reverse integration of interpretability analysis results into feature engineering or model optimization. Third, enhance accuracy through multi-wavelength joint calibration and dynamic refractive index compensation algorithms.

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