

A Precise Measurement of Semiconductor Epitaxial Layer Thickness Based on a Hybrid Refractive Index Model and Fourier Transform Correction

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Abstract: This paper aims to address the core issue of accurately determining the epitaxial layer thickness of silicon carbide (SiC) semiconductors using infrared interference spectroscopy, particularly in response to challenges posed by missing spectral data and multiple-beam interference effects. The study first establishes a physical model based on the principle of two-beam interference and innovatively introduces the Drude-Sellmeier hybrid model to precisely characterize the dispersion and free carrier effects of SiC materials. To resolve the problem of missing interference fringes in the phonon resonance region, a "global interference order alignment" algorithm is designed, which initially determines the epitaxial layer thickness through global optimization. Furthermore, to eliminate the systematic impact of multiple-beam interference on measurement accuracy, a correction model based on fast Fourier transform (FFT) is proposed. Experimental results show that for silicon (Si) wafers with significant multiple-beam interference, the FFT method dramatically reduces the relative measurement difference at different incident angles from 1.671% to 0.1512%; when applied to SiC samples, this method also optimizes the relative measurement difference from 1.3129% to 0.4396%, ultimately determining the epitaxial layer thickness to be 11.16 μm . The analysis framework established in this paper, from initial optimization to FFT correction, provides an effective methodology for high-precision, highly robust, nondestructive epitaxial layer thickness measurement.

Keywords: Epitaxial layer thickness, fast Fourier transform, global optimization, Drude-Sellmeier hybrid model, multi-beam interference.

1. Introduction

Silicon carbide (SiC), as an outstanding representative of third-generation wide bandgap semiconductors, demonstrates tremendous application potential in cutting-edge fields such as RF communications, new energy vehicles, and power electronics, thanks to its excellent physical properties including high breakdown electric field, high thermal conductivity, and high electron saturation velocity[1,2]. Among the many critical parameters of epitaxial materials, the thickness of the epitaxial layer directly affects device breakdown voltage, capacitance characteristics, and overall performance. Therefore, establishing a scientific, accurate, and reliable non-destructive method for thickness measurement is crucial for ensuring device quality and driving industry development[2]. The infrared reflectance spectral interference method, due to its non-contact and non-destructive nature, has become the standard technique for characterizing epitaxial layer thickness[3, 4]. The core challenge of this technique lies in how to accurately extract a unique thickness value from the interference spectrum, which may contain noise, missing signals, and complex physical effects.

Currently, thickness calculation methods based on infrared interference spectra primarily rely on analyzing the extremum points of interference fringes. Traditional methods estimate thickness by examining the spacing of adjacent interference fringes. However, these methods often prove inadequate when faced with practical challenges[5].

To address these shortcomings, this paper proposes a progressive analytical framework, advancing from initial optimization to precise correction. The distinctive features

and contributions of this work are, first, the design of a "global interference order alignment" algorithm that does not rely on fringe continuity and can effectively address the issue of missing interference signals caused by phonon absorption through global numerical optimization[6].

The structure of this paper is organized as follows: First, the methods section presents a detailed explanation of the underlying physical models for thickness measurement, including the principles of two-beam interference and the Drude-Sellmeier mixed refractive index model, and sequentially introduces the key concepts and implementation paths of the "global interference order alignment" algorithm and the Fourier transform correction model. Next, in the results and analysis section, the effectiveness of the proposed method is validated step by step using SiC and Si wafers as examples, with in-depth interpretation of the results. Finally, the conclusion section summarizes the work of this paper, and discusses the advantages, limitations, and future research directions of the model.

2. Methods

2.1. Theoretical Model Foundation

The epitaxial layer thickness measurement model constructed in this study is theoretically based on the interference principle of thin film optics. When an infrared beam enters at a specific incident angle, reflected light is generated at both the air-epitaxial layer interface and the epitaxial layer-substrate interface. In an ideal two-beam interference model that considers only first-order reflections, these two coherent beams produce an optical path difference due to their different propagation paths.

Through geometric optics derivation, and by taking into account the half-wavelength loss caused by reflection at interfaces with higher refractive indices[7], the core relationship for the condition of destructive interference (i.e., when valleys appear in the reflection spectrum) can be established.

$$\Delta s = 2n_2x \cos \beta_2 = 2x\sqrt{n_2^2 - \sin^2 \beta_1} \quad (1)$$

Δs : Optical path difference (the difference in optical path lengths traveled by the two coherent reflected beams);

x : Epitaxial layer thickness (target measurement parameter);

n_2 : Refractive index of the epitaxial layer (varies with wavenumber and material properties like carrier concentration);

β_1 : Incident angle of the infrared beam (a specified parameter in the measurement experiment);

β_2 : Refraction angle of the infrared beam.

$$2x\sqrt{n_2(\sigma_j, \rho_1)^2 - \sin^2 \beta_1} = \frac{j}{\sigma_j} \quad (2)$$

σ_j : Wavenumber at the j -th destructive interference (extracted from the experimental reflection spectrum);

j : Interference order (a positive integer indicating the order of the interference fringe);

ρ_1 : Carrier concentration of the epitaxial layer (affects the refractive index n_2 via free carrier effects);

x : Epitaxial layer thickness (target measurement parameter);

n_2 : Refractive index of the epitaxial layer (varies with wavenumber and material properties like carrier concentration);

β_1 : Incident angle of the infrared beam (a specified parameter in the measurement experiment).

This relationship links the epitaxial layer thickness to be measured, the refractive index of the epitaxial layer, the incident angle, the wavenumber at which destructive interference occurs, and the corresponding interference order (a positive integer).

To ensure the accuracy of the model, it is essential to precisely describe the variation of the refractive index of the epitaxial layer with wavenumber and material properties. Considering that both lattice vibrations and free carriers in SiC material have significant effects on optical constants, this study adopts a Drude-Sellmeier hybrid model[8, 9].

$$\varepsilon_{total}(\sigma) = \varepsilon_{lattice}(\sigma) + \varepsilon_{carrier}(\sigma) \quad (3)$$

$\varepsilon_{total}(\sigma)$: Total complex permittivity of the SiC epitaxial layer as a function of wavenumber σ ;

$\varepsilon_{lattice}(\sigma)$: Permittivity contribution from lattice vibrations (described by the Sellmeier equation);

$\varepsilon_{carrier}(\sigma)$: Permittivity contribution from free carriers (described by the Drude model);

σ : Wavenumber of the incident infrared light.

$$\varepsilon_{lattice}(\sigma) = A + \sum_i \frac{B_i \sigma_i^2}{\sigma_i^2 - \sigma^2} \quad (4)$$

A, B_i, σ_i : Material-specific Sellmeier coefficients (obtained from literature or fitting for SiC);

σ : Wavenumber of the incident infrared light.

$$\varepsilon_{carrier}(\sigma) = -\frac{\omega_p^2}{\omega^2 + i\gamma\gamma} \quad (5)$$

$\omega = 2\pi c\sigma$: Angular frequency of the infrared light (with c being the speed of light in vacuum);

$$\omega_p^2 = \frac{\rho e^2}{\varepsilon_0 m^*}$$

: Square of the plasma frequency (where ρ is carrier concentration, e is electron charge, ε_0 is vacuum permittivity, m^* is effective carrier mass);

γ : Damping factor (related to carrier scattering in the material);

σ : Wavenumber of the incident infrared light.

$$n_2(\sigma, \rho_1) = \sqrt{\frac{\text{Re}(\varepsilon_{total}) + \sqrt{\text{Re}(\varepsilon_{total})^2 + \text{Im}(\varepsilon_{total})^2}}{2}} \quad (6)$$

n_2 : Refractive index of the epitaxial layer (varies with wavenumber and material properties like carrier concentration);

ρ_1 : Carrier concentration of the epitaxial layer (affects the refractive index n_2 via free carrier effects);

σ : Wavenumber of the incident infrared light;

$\text{Re}(\varepsilon_{total})$: Real part of the total complex permittivity (of the SiC epitaxial layer);

$\text{Im}(\varepsilon_{total})$: Imaginary part of the total complex permittivity (of the SiC epitaxial layer).

2.2. Global Interference Order Alignment Algorithm

Traditional methods for calculating thickness use consecutive interference minima. However, this doesn't work when data is missing, like in the SiC phonon resonance area. To solve this, the paper introduces a new algorithm called "global interference order alignment."

$$j'(x) = 2x\sigma_j \sqrt{n_2(\sigma_j, \rho_1)^2 - \sin^2(\beta_1)} \quad (7)$$

$j'(x)$: Theoretical interference order (should be close to an integer for the true thickness x);

x : Epitaxial layer thickness (the physical quantity to be measured in this study);

σ_j : Wavenumber at the j -th destructive interference;

n_2 : Refractive index of the epitaxial layer (varies with wavenumber and material properties like carrier concentration);

ρ_1 : Carrier concentration of the epitaxial layer (affects the refractive index n_2 via free carrier effects);

β_1 : Incident angle of the infrared beam (a specified parameter in the measurement experiment).

This algorithm doesn't rely on the closeness of minima points. Instead, it focuses on the basic interference condition: for a true thickness, the theoretical interference order at any observed minimum should be close to a whole number. We change the thickness problem into a one-dimensional numerical optimization problem. First, we adjust the main interference relationship to get a formula for calculating the theoretical interference order, which depends on thickness and wavenumber. Then, we create an objective function to measure how much the calculated interference orders at observed minima differ from whole numbers for a given thickness.

$$E(x) = \sum_{j=1}^k (j'(x) - \text{round}(j'(x)))^2 \quad (8)$$

$E(x)$: Total deviation between theoretical interference orders and their nearest integers (smaller $E(x)$ = better consistency);

$j'(x)$: Theoretical interference order (should be close to an integer for the true thickness x);

$\text{round}(\cdot)$: Rounding function (returns the nearest integer to $j'(x)$);

k : Number of detected interference minima in the spectrum.

The goal is to find the thickness that makes this difference as small as possible. This algorithm uses all valid data points and works well even if some interference fringes are missing.

$$x^* = \arg \min_x E(x) \quad (9)$$

x^* : Optimal epitaxial layer thickness (solution that minimizes $E(x)$, constrained to a physical range, e.g., 5–18 μm for SiC);

$E(x)$: Total deviation between theoretical interference orders and their nearest integers (smaller $E(x)$ = better consistency).

In practice, we first smooth the raw spectral data using a Savitzky-Golay filter to remove noise. Then, we use a local minima search to find all interference minima points. Finally, we use a one-dimensional bounded optimizer to find the best thickness within a reasonable range.

2.3. Multi-beam Interference Identification and FFT Correction Model

The "global interference order alignment" algorithm helps with missing data, but it needs to find interference valley points accurately. If the interface reflectivity is high or material absorption is low, multiple-beam interference can happen. This changes the interference pattern from a smooth wave to a sharp pulse[10]. This shift causes a mismatch between the calculated and actual interference points, affecting the algorithm's accuracy. To check for multiple-beam interference, the paper uses kurtosis, a measure of how sharp a signal is. For a perfect two-beam interference, kurtosis is 1.5. If the kurtosis of the interference signal is much higher

than 1.5, it means multiple-beam interference is present[10, 11].

$$k = \frac{E[(y_2 - \mu)^4]}{\varsigma^4} \quad (10)$$

k : Kurtosis of the interference signal (≈ 1.5 for ideal two-beam interference; much higher values indicate multi-beam interference);

$y_2(\sigma)$: Interference oscillation signal (raw spectrum with baseline removed);

$E[\cdot]$: Expectation operator (average over the wavenumber domain);

μ : Mean of $y_2(\sigma)$;

ς : Standard deviation of $y_2(\sigma)$.

To fix errors from changes in fringe shape, the paper suggests a correction model using Fast Fourier Transform (FFT). This method works because the interference spectrum's "instantaneous frequency" is linked to the optical path difference. By applying FFT, the interference spectrum is changed from the wavenumber domain to the optical path difference domain. In this new spectrum, a clear peak shows the average optical path difference[12]. Using this and the average refractive index, a more accurate layer thickness can be found, unaffected by fringe shape[12].

$$x = \frac{\overline{\Delta s}}{2\sqrt{n_2^2 - \sin^2 \beta_1}} \quad (11)$$

$\overline{\Delta s}$: Average optical path difference (obtained from the peak of the FFT-transformed spectrum);

n_2 : Average refractive index of the epitaxial layer (integrated over the measurement wavenumber range);

x : Corrected epitaxial layer thickness (unaffected by multi-beam interference);

β_1 : Incident angle (defined in Snell's Law).

This method doesn't need to find local extrema and avoids multiple-beam interference issues.

3. Results

3.1. Preliminary Calculation and Model Validation for SiC Epitaxial Layer Thickness

In this study, the "Global Interference Order Alignment" algorithm was first applied to the spectral data of silicon carbide wafers provided in Appendix 1 (incident angle 10°) and Appendix 2 (incident angle 15°). As shown in Figure 1, after Savitzky-Golay smoothing, the algorithm successfully identified 22 and 23 significant interference minima in the two data sets, respectively. These points are mainly distributed in the pronounced oscillation region of 500–2000 cm^{-1} . By optimizing the objective function, the calculated epitaxial layer thickness was 10.2912 μm at a 10° incident angle and 10.4272 μm at a 15° incident angle. The average thickness of the two measurements was 10.3592 μm , with a relative difference of 1.3129% between them.

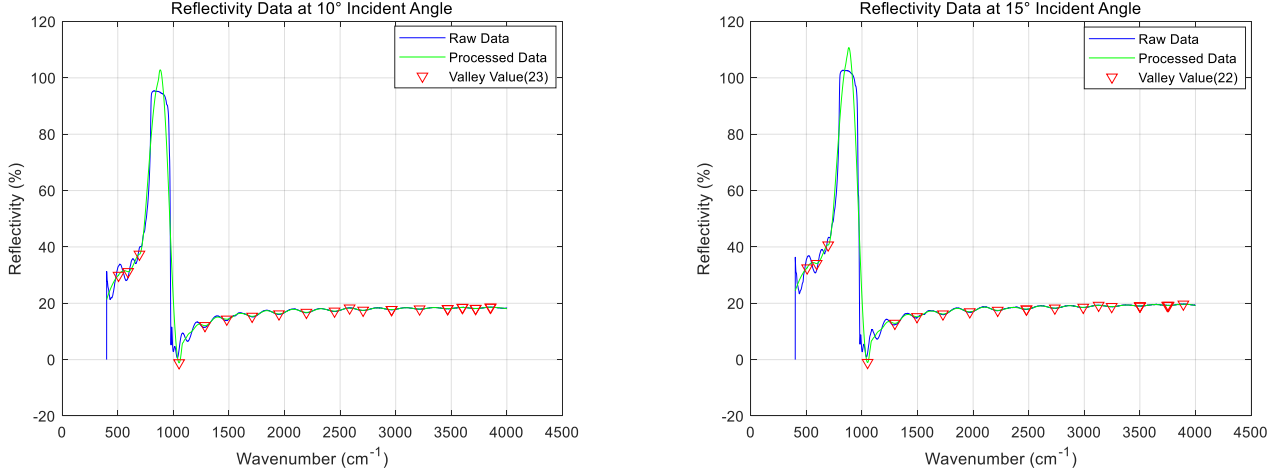


Figure 1. Smoothing and localization of interference minima in the reflectance spectra of silicon carbide

To evaluate the effectiveness of the model, we introduced a diagnostic plot of global interference order alignment for analysis, as shown in Figure 2. The figure illustrates that, for both incident angles, the theoretically calculated interference orders based on the optimal thickness were tightly clustered near their respective integer orders, with root mean square errors of approximately 0.16. This indicates a minimal deviation between the calculated theoretical values and the

ideal integer values. This result strongly validates both the physical model established in this paper and the logical accuracy of the "global alignment" algorithm. However, the 1.3129% difference between the two independent measurement results suggests the existence of systematic effects that may not have been fully considered in the model, prompting further investigation into the potential influence of multiple-beam interference.

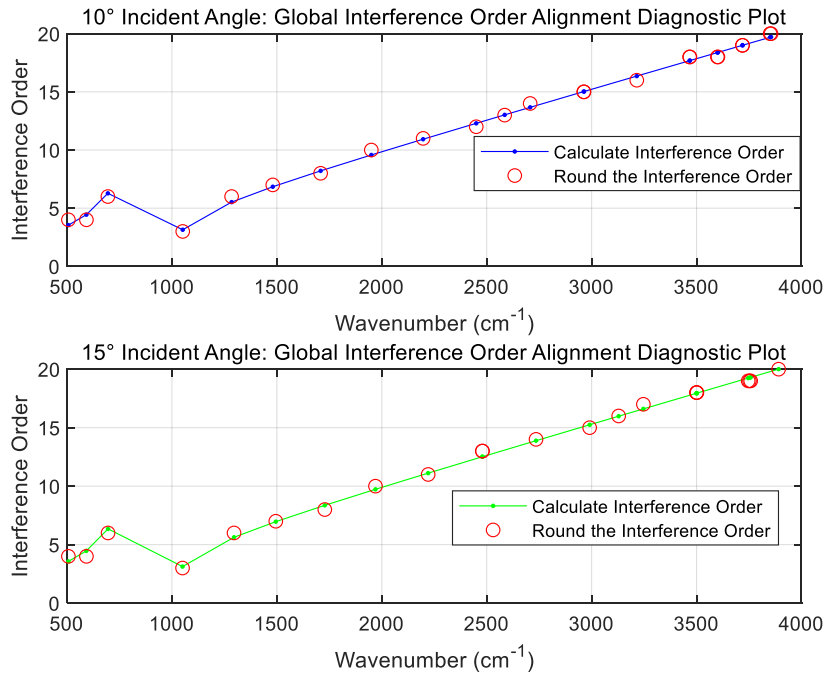


Figure 2. Global interference order alignment diagnostic plot at incident angles of 10° and 15°

3.2. Identification of Multi-beam Interference Effects and Analysis of Algorithmic Limitations

To verify the interference of multiple-beam effects on the extremum-based positioning algorithm, this paper uses the silicon wafer data provided in Appendix 3 and Appendix 4 as reference cases under strong interference. Silicon, with its low absorption rate in the infrared band and significant refractive

index contrast at interfaces, is an ideal system for generating pronounced multiple-beam interference. As shown in Figure 3, we first extract the pure interference oscillation signal using the baseline separation method and then calculate its kurtosis. The results show that, at incident angles of 10° and 15°, the kurtosis values of the spectral oscillations reach 5823 and 5948, respectively—three orders of magnitude higher than the theoretical value of 1.5 for ideal two-beam interference. This

result quantitatively and unequivocally confirms the presence of extremely strong multiple-beam interference in the spectra

of silicon wafers, leading to highly sharp, non-sinusoidal interference fringes.

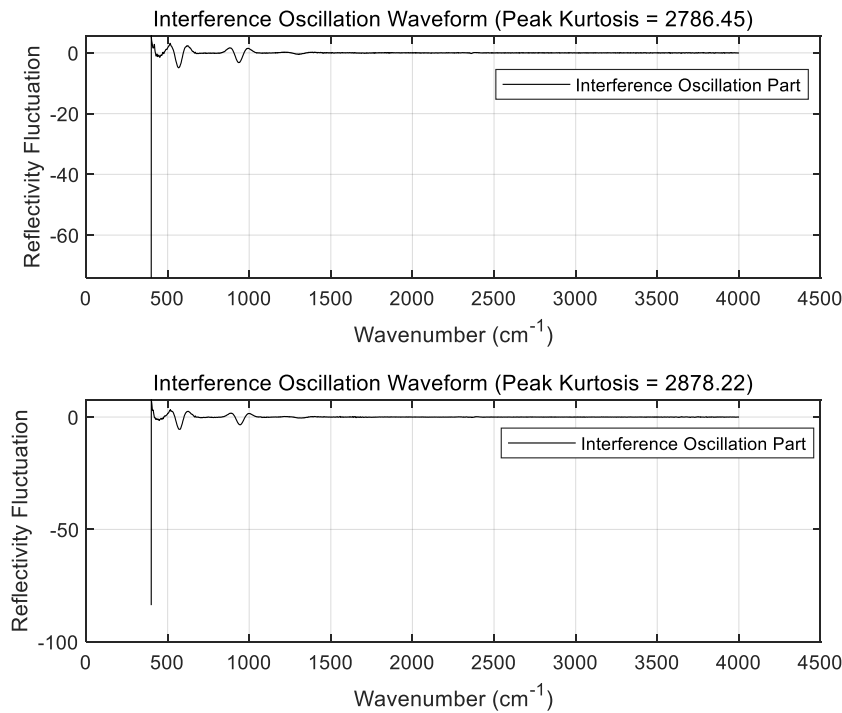


Figure 3. Interference oscillation waveform and high-kurtosis features of silicon wafers

Subsequently, we applied the “global interference order alignment” algorithm to this set of silicon data, which exhibits strong multiple-beam interference. The calculated thicknesses at incident angles of 10° and 15° are $19.6748\ \mu\text{m}$ and $19.3667\ \mu\text{m}$, respectively, with a relative difference of 1.671%. This difference, which is significantly greater than that observed in the silicon carbide samples, indicates that when interference fringes are severely distorted by the multiple-beam effect, the systematic deviation between the mathematical minima identified by the peak-finding algorithm and the physical phase points is amplified, leading to a considerable decline in the accuracy and consistency of the algorithm. This case clearly reveals the inherent limitations of the “global interference order alignment” algorithm when processing data with strong multiple-beam interference.

3.3. Thickness Calculation Optimization Based on Fourier Transform and Final Results

To overcome the above-mentioned limitations, this study introduces a modified model based on the Fourier Transform (FFT). The FFT method is applied to the silicon wafer data, transforming the spectral signal from the wavenumber domain to the optical path difference domain. In the resulting power spectrum, a sharp and positionally stable main peak appears, which directly corresponds to the average optical path difference of the sample. Based on the location of this peak, the calculated thickness of the silicon epitaxial layer is $11.7698\ \mu\text{m}$ and $11.7876\ \mu\text{m}$ at incident angles of 10° and 15° , respectively, with a relative difference of only 0.1512%. Compared to the previous 1.671%, the consistency of the results has improved by more than an order of magnitude, fully demonstrating that the FFT method can effectively immunize against the interference of weak multi-beam effects on fringe shape, thus providing precise and reliable

measurement results.

After confirming the superiority of the FFT method, we applied it to the original silicon carbide data to correct for possible weak multi-beam interference effects. The kurtosis analysis of the silicon carbide spectrum showed kurtosis values of about 12 to 16, which is also significantly higher than 1.5, confirming the presence of weak multi-beam interference. After recalculating with the FFT method, the thickness of the silicon carbide epitaxial layer was determined to be $11.1487\ \mu\text{m}$ and $11.1836\ \mu\text{m}$ at 10° and 15° , respectively. The relative difference between the two measurements decreased to 0.4396%, indicating a significant improvement in consistency. This result shows that the differences observed in the initial algorithm were indeed caused by systematic interference from weak multi-beam effects on the positioning of extremum points. Ultimately, we took the average of the two highly consistent FFT measurement results and determined the thickness of the silicon carbide epitaxial layer to be $11.16\ \mu\text{m}$, which represents the best estimate under the modified model proposed in this study.

4. Conclusions

This paper successfully establishes and validates a progressive analytical framework for the precise measurement of semiconductor epitaxial layer thickness. The core contribution lies in proposing effective solutions to two major challenges in infrared interference spectroscopy analysis: data loss and multiple-beam interference effects. First, based on an accurate Drude-Sellmeier hybrid refractive index model, a “global interference order alignment” algorithm was developed. Through global optimization, this algorithm efficiently overcomes the problem of missing interference fringes caused by strong material absorption. Subsequently, kurtosis analysis is introduced to quantitatively

identify multiple-beam interference, and on this basis, a fast Fourier transform (FFT) correction model is applied. This fundamentally eliminates systematic errors introduced by changes in interference fringe patterns, significantly improving the precision and consistency of measurement results.

The FFT correction model presented in this study demonstrates outstanding robustness and accuracy. Its advantage lies in extracting thickness information directly from the global frequency characteristics of the spectrum, thereby completely avoiding reliance on the morphology of local extrema. However, the overall accuracy of the model still depends on the precision of the physical parameters used in the Drude-Sellmeier model (such as Sellmeier coefficients, effective mass of carriers, etc.). These parameters are typically obtained from literature references, which may introduce uncertainty.

Future research directions may focus on further optimizing the algorithm and model. On the one hand, the optimization process for thickness determination can be integrated with the fitting of key parameters in the refractive index model, achieving simultaneous inversion of both thickness and optical constants, thereby reducing dependence on a priori parameters. On the other hand, the analytical approach from this study—particularly the application of FFT methods—can be extended to more complex multilayer film systems. By combining with optical transfer matrix theory, this would provide a more powerful analytical tool for structural characterization of multilayer semiconductor devices.

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