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Improvement of Reflectance Spectroscopy for Oxide Layers on 4H-SiC

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Abstract. In this work, we investigate the use of reflectance spectroscopy as an accurate, fast, and non-destructive method for measuring the thickness of transparent layers, such as SiO_2, with thicknesses below 200 nm for microelectronic applications. To this end, we fabricated different oxides and analyzed their reflectance spectra using reflectance spectroscopy. The results were compared to theoretical reflectance spectra to validate the method. We introduce key factors to ensure accurate measurement by modeling the reflectance spectra of thin oxide layers with thicknesses ≥ 15 nm on 4H-SiC using the transfer matrix method (TMM).

Introduction

Due to the more suitable properties for high voltage, high frequency and high temperature applications of silicon carbide (SiC) compared to silicon (Si), SiC is increasingly replacing Si semiconductor devices, especially in power applications [1]. Most steps during the device fabrication process involve the formation and structuring of transparent layers on SiC. These layers can be either deposited or grown by using different techniques, e.g., thermal oxidation, plasma-enhanced chemical vapor deposition (PECVD), among others [2]. Each layer is defined by its physical and chemical properties, which can be characterized by a variety of established and commercially available methods such as stylus profilometry, eddy current, x-ray reflectance, ellipsometry, reflectance spectroscopy, or various other techniques [3–5]. Since the properties of these deposited layers often strongly depend on their actual thickness, it is of utmost importance to reliably characterize this parameter. The most commonly used techniques for thickness characterizations are optical methods, mainly because of their advantages such as high measurement resolution, their non-destructive and non-contact character [6]. Due to its smaller spot-sizes and lower costs compared to ellipsometry, microscope-based reflectance spectroscopy has attracted considerable attention and is, therefore widely established in the semiconductor industry.

Reflectance spectroscopy is usually based on the illumination of a sample with a beam of white light, the measurement of the reflectance spectrum with a spectrometer and the evaluation with theoretical models mostly based on the transfer-matrix method [7]. In order to obtain reliable thickness data using reflectance spectroscopy, the knowledge of the optical constants consisting of the refractive index (n) and the extinction coefficient (k) is crucial. The optical constants of SiC are strongly dependent on the SiC polytype, its dopant type, e.g. nitrogen (N) or aluminum (Al), and its doping concentration [8–11]. In general, the transparent properties of the SiC in the spectrum of white light also need to be taken into account. Therefore, a proper evaluation of thin oxides such as gate oxides and sacrificial oxide using reflectance spectroscopy on 4H-SiC substrates must take into account all relevant aspects. Their influence will be investigated exemplarily.

Experiment

In this study, theoretical reflectance spectra were investigated to understand the impact of the SiC substrate properties, especially the substrate doping and its transparent properties, on the thickness measurement of the transparent layers applied on top of it. For the investigation, two different oxides were grown on commercially available, highly conductive n-type (by N doping) 4° off-axis 4H-SiC substrates (0001) with standard specifications by dry oxidation in O_2 followed by annealing in NO. One substrate was oxidized at 1300 °C , which corresponds to our typically used gate oxide for SiC-MOSFETs and the other substrate was oxidized at 1150 °C in order to grow a sacrificial oxide. The target-thicknesses of these oxides on the Si-face were 60 nm for the gate oxide and 5 nm for the sacrificial oxide, respectively 130 nm (gate oxide) & 15 nm (sacrificial oxide) on the C-face. Due to the different oxide growth rates on the (0001) Si-face and the $(000\bar{1})$ C-face the thickness of the oxides on the C-face deviate from the target thickness of the Si-face [2]. After processing, the oxides were characterized by spectroscopic ellipsometry (Horiba AutoSE), as well as by reflectance spectroscopy (K-Mac ST5030-SL), and compared to theoretical reflectance spectra calculated using the 2x2 transfer matrix method, as implemented in the software created by Schwarz et al. [12]. The results from spectroscopic ellipsometry were used as the reference for comparison with the experimental and theoretical reflectance spectra. To perform this calculation, we assumed optical layer stacks with n homogeneous isotropic layers on a semi-infinite substrate, on which an incident polychromatic light beam was partially reflected and partially transmitted at every layer interface, and in case of the 4H-SiC layer, some of the light was partially absorbed within the layer. The optical constants used for the modelling of SiO_2 were taken from Maliton [13], and the optical constants of 4H-SiC were taken from 4H-SiC Khadivianazar et al. [14]. Moreover the thick 4H-SiC substrate was modeled by assuming that it was incoherent, according to [15]. For the reflectance spectroscopy measurement, the sample was illuminated with a collimated beam of light using a 5x/NA 0.10 objective lens. The reflected light was then split into two beams by a beam splitter. One beam was focused onto a CCD camera for imaging, while the other beam was coupled into a glass fiber and analyzed by a spectrometer. The spectral range of the measurement was 400 to 800 nm. The measured reflectance spectra were compared to the modeled spectra by calculating the residual sum of squares (RSS) over the evaluated wavelength range, which was calculated as follows:

$$\mathrm{RSS} = \sum_{\lambda_{\min}}^{\lambda_{\max}} \frac{[R_{\mathrm{meas}}(\lambda) - R(\lambda)]^2}{M}, \tag{1}$$

where $R_{means}(\lambda)$ are the measured reflectance values at each wavelength λ of the spectrum, $R(\lambda)$ are the modeled reflectance values at each wavelength λ of the spectrum and M is the number of measurement points within the boundaries λ_{min} and λ_{max}.

Results

Fig. 1 shows the theoretical reflectance spectra for various SiO_2 films on a 350 µm 4H-SiC substrate with SiO_2 thickness values of 10, 20, 50, 100 and 200 nm. For this, the SiO_2 films and the 4H-SiC substrate were modeled as homogeneous isotropic layers on a semi-infinite substrate of air. The reflectance spectra for all SiO_2 films with thicknesses $\leq$ 50 nm show no distinct interference extrema, unlike thicker films. Instead, the reflectance spectra are mainly influenced by the absorption in 4H-SiC due to the electronic transition from the dopant band to the higher conduction band at wavelengths of 460 and 570 nm [8,9]. This results in a similar shape for all spectra, with distinctive minima near these wavelengths. However, the absolute reflectance values are different for different thicknesses. This suggests that for thicknesses $\leq$ 50 nm, the SiO_2 layer does not cause any interference between the transmitted and reflected light, but rather acts as an anti-reflection coating, which is thickness dependent. This difference in the reflectance can be determined by reflectance spectroscopy if the reflectance difference is large enough to be detected by the spectrometer. The reflectance of a 10 nm SiO_2 layer on a 4H-SiC substrate is 0.8 % lower than that of the bare substrate at 400 nm. The reflectance difference decreases with increasing wavelength, making it difficult to detect. However, the reflectance difference of 3.2 % for a 20 nm SiO_2 layer is larger and should be detectable. This demonstrates the general feasibility of measuring ultra-thin oxide layers with thickness $\geq$ 20 nm and indicate the impact of the N doping of the SiC substrate on SiO_2 films with thicknesses $\leq$ 50 nm.

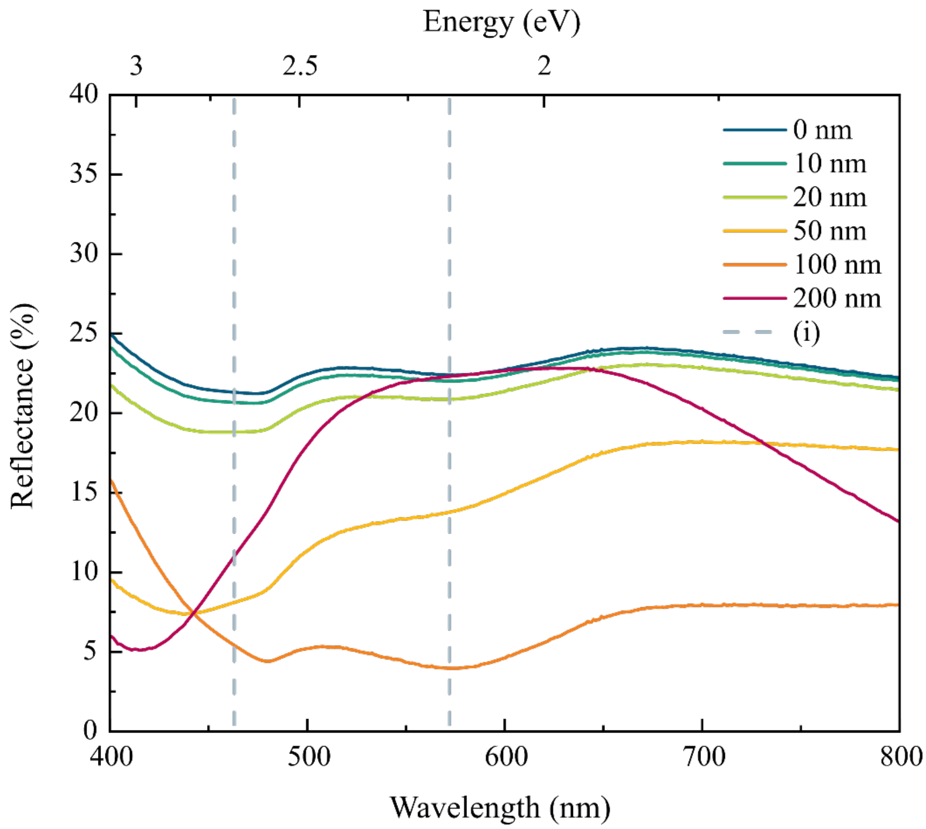

Fig. 1 Theoretical reflectance spectra of Air / SiO_2 / 350 µm SiC / Air layer stacks over the 400–800 nm spectral range and for SiO_2 thicknesses in the 0–200 nm range, with the optical constants of an 18.3 mΩ·cm 4H-SiC sample [13,14]. The vertical lines (i) show electronic transition wavelengths for dopant band to higher conduction band transitions in the 4H-SiC substrate [8,9].

The reflectance spectra of n-type (by Nitrogen-dope) 4H-SiC substrate with a nominal specific resistivity of 18.0 mΩ·cm (specification provided by the supplier) and of a total thickness of 356 µm with a 60.1 nm thick SiO_2 layer grown by dry oxidation on the Si-face and a 130.3 nm thick SiO_2 layer on the C-face is presented in Fig. 2. The thickness of the SiO_2 layer was obtained by spectroscopic ellipsometry and compared to modeled reflectance spectra generated for three different layer stacks calculated with the obtained thicknesses: (1) Air /SiO_2 / 4H-SiC (semi-infinite), (2) Air / SiO_2 / 4H-SiC / Air (semi-infinite), and (3) Air / SiO_2 / 4H-SiC / SiO_2 / Air (semi-infinite). From the results obtained via the 2x2 transfer matrix method the modeled Air / SiO_2 / 356 µm SiC / 130.3 nm SiO_2 / Air (Model 2) matches best to the measured values with an RSS of 1.1×10^{-5} compared to Model 1 with a RSS of 9.5×10^{-5} and Model 2 with 63.3×10^{-5}. This shows the necessity for the additional modelling of the backside reflection of the 4H-SiC substrate as well as the reflection based on the SiO_2 on the C-face to obtain accurate theoretical reflectance spectra.

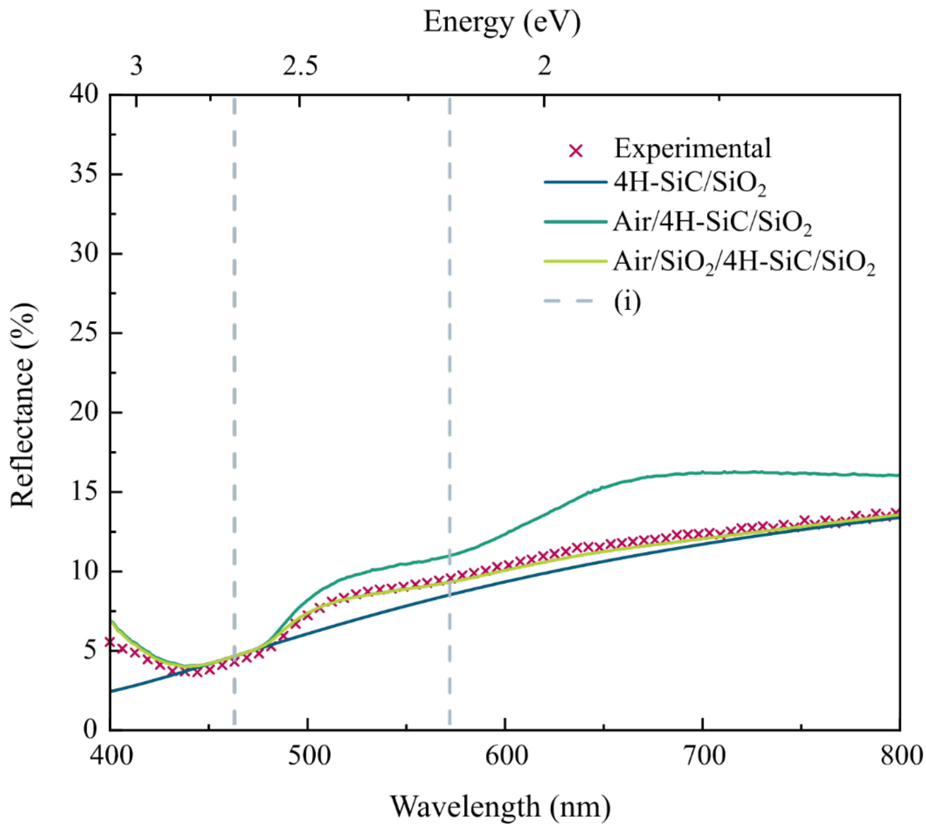

Fig. 2 Experimental reflectance spectrum of Air / 60.1 nm SiO_2 / 356 µm n-type 4H-SiC (18 mΩ·cm) / 130.3 nm SiO_2 / Air compared to calculated spectra using different layer stacks with the optical constants of [13] and an 18.3 mΩ·cm 4H-SiC sample [14]. Vertical lines (i) show dopant band to higher conduction band transition wavelengths [8,9].

Taking these factors into account, Fig. 3a shows the reflectance spectra of a n-type (N-doped) 4H-SiC substrate which has a specific resistivity of 17.9 mΩ·cm. The reflectance spectra of the substrate, which has 16.2 nm oxide on the C-face and 5.7 nm on the Si-face, is compared to theoretical reflection spectra based on different optical constants of n-type 4H-SiC substrates with different substrate resistivities such as 18.3 mΩ·cm, 21.5 mΩ·cm, and 24.7 mΩ·cm [14]. For the modeling, the backside reflection of the 4H-SiC substrate (343 µm) and the reflection based on the SiO_2 on the C-face were both considered. The SiO_2 thickness has been obtained by spectroscopic ellipsometry. In comparison the calculated reflectance spectrum obtained with the optical constants from a 18.3 mΩ·cm 4H-SiC sample fits best to the measured data with a RSS of 11.7×10^{-5}. This is compared to the reflectance spectra obtained with the optical constants from 21.5 mΩ·cm with an RSS of 981.7×10^{-5} and 24.7 mΩ·cm with an RSS of 219.0×10^{-5}, respectively. To validate the accuracy of our model, the residual sum of squares of the experimental and theoretical spectra with the same optical constants from Khadivianazar et al. used in Fig. 3a are plotted in Fig. 3b. The RSS values for the 18.3 mΩ·cm, 21.5 mΩ·cm, and 24.7 mΩ·cm all show a distinctive minimum at different thicknesses. However, only the RSS based on the model with the optical constant, close to the one of the measured sample, from an 4H-SiC n-type substrate with the resistivity of 18.3 mΩ·cm show a minimum at 16 nm which agrees with the measured ellipsometer data. In contrast to this the minima of the RSS for the modelling using the 21.5 mΩ·cm is at 24 nm and for the 24.7 mΩ·cm modelling at 31 nm. The difference in the minima of the RSS values for the different models is due to the varying absorption of the 4H-SiC substrates with different N-dopant concentrations, which is reflected in a difference in the resistivity. This is because the absorption coefficient of 4H-SiC increases with increasing N-dopant concentration [14]. The precise knowledge of the n, k values for different doping concentrations is therefore paramount in order to accurately model and evaluate reflectance spectra of transparent layers, such as SiO_2 on 4H-SiC.

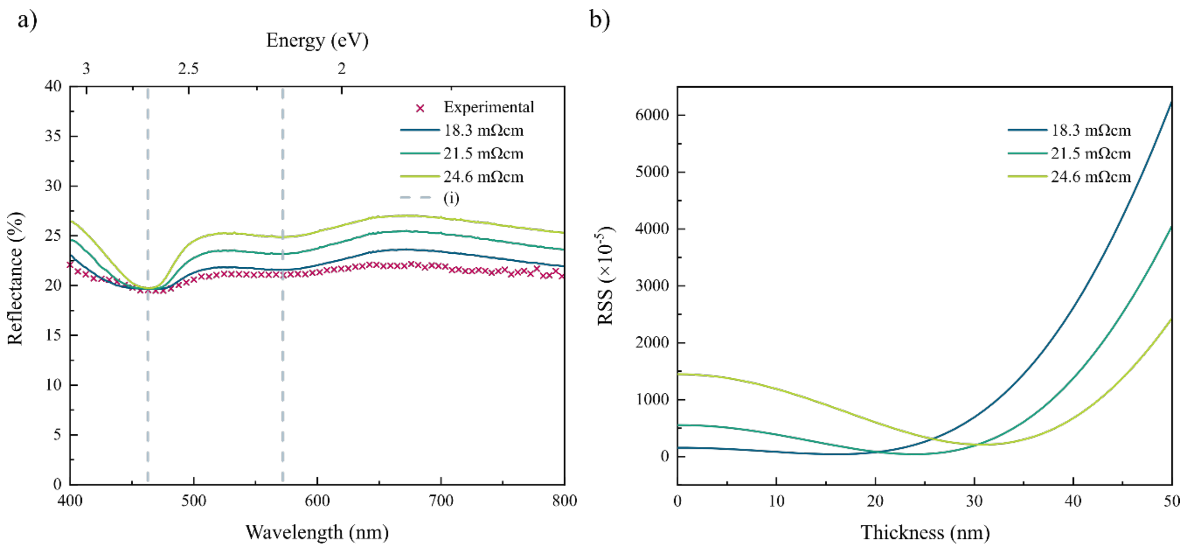

Fig. 3a Experimental reflectance spectrum of 16.2 nm SiO_2 / 343 µm n-type 4H-SiC (17.9 mΩ·cm) / 5.7 nm SiO_2 / Air compared to theoretical spectra varying the optical constants of the 4H-SiC from [13] for the following resistivity 18.3 mΩ·cm, 21.5 mΩ·cm and 24.7 mΩ·cm. Vertical lines (i) show dopant band to higher conduction band transition wavelengths [8,9]. Fig. 3b RSS from 0 to 50 nm of the experimental and theoretical spectra for different 4H-SiC optical constants from [14].

The good agreement between the theoretical reflection spectra based on optical constants of a n-type 4H-SiC substrate with the substrate resistivities of 18.3 mΩ·cm and the measured sample, in combination with the additional modeling of the backside reflection of the 4H-SiC substrate and the reflection based on the SiO_2 on the C-face, demonstrates the possibility of measuring even thin oxide layers (≥ 15 nm thickness).

Summary

This work discusses important factors to be considered when optimizing the modeling and measurement of thin transparent layers on 4H-SiC substrates using reflectance spectroscopy. One important factor is the semi-transparent nature of 4H-SiC, which requires the additional modelling of the backside reflection of the 4H-SiC substrate as well as the reflection based on the layers on the C-face of the wafer. Additionally, the impact of the N-dopant concentration on the optical constants must be taken into account. This requires the precise knowledge of the n, k values for different doping concentrations in order to accurately model and evaluate reflectance spectra of transparent layers on 4H-SiC. Provided that all the aforementioned factors are considered, then even ultra-thin oxide layers on 4H-SiC with thicknesses of ≥ 15 nm can be determined by reflectance spectroscopy.

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