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Decoupling of silicon carbide optical sensor response for temperature and pressure measurements

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Decoupling of silicon carbide optical sensor response for temperature and pressure measurements

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Single crystal silicon carbide is a chemically inert transparent material with superior oxidation-resistant properties at elevated temperatures compared to black polycrystalline silicon carbide substrates. These improved properties make crystalline silicon carbide a good optical sensor material for harsh environments such as combustion chambers and turbine systems. Interferometric optical sensors are orders of magnitude more sensitive than electrical sensors and are proposed for these applications. Silicon carbide itself behaves as a Fabry-Pérot etalon eliminating the need for an external interferometer for any measurement using this silicon carbide as a sensor. The principle of the optical sensor in this study is the temperature- and pressure-dependent refractive index of silicon carbide, which can be used to determine the temperatures and pressures of gases that are in contact with silicon carbide. Interference patterns produced by a silicon carbide (4H-SiC) wafer due to multiple reflections of a helium-neon laser beam of wavelength of 632.8 nm have been obtained at temperatures up to 500 °C and pressures up to 600 psi. The pattern changes for the same gas at different temperatures and pressures and for different gases at the same temperature and pressure. The refractive index at the wafer-gas interface is calculated from the interference pattern and the refractive index gradients with respect to temperature and pressure, respectively, are also determined. Decoupling temperature and pressure using these gradients and the measured reflectivity data are discussed in this paper. © 2007 American Institute of Physics.

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I. INTRODUCTION

The high temperature, high pressure, and harsh chemical environments of combustion chambers and turbine systems in power plants require remote sensing capability for online control and monitoring of the system components. Owing to better mechanical strength, thermal stability, and chemical inertness of silicon carbide (SiC) than many other dielectric materials, SiC can be used as an optical device for remote sensing applications. Compared to conventional electronic sensors, optical sensors have many advantages including small size, light weight, high sensitivity, large bandwidth, high reliability, immunity to electromagnetic interference, corrosion and oxidation resistance, and the absence of spark hazard in inflammable environments.¹ Optical sensors can also survive at much higher temperatures than conventional pressure sensors.²

The aerospace and automotive industries require optical sensors that can operate at high temperatures and pressures under potentially corrosive and harsh conditions.^{3,4} For operations at temperatures greater than 300 °C and in harsh

environments, SiC sensors have been employed. The wide band gap (3.2 eV for 4H-SiC), high thermal conductivity, and high chemical stability make SiC a gas sensing material of choice for extreme environments.⁵⁻⁷ Strong affinity of SiC to hydrocarbons makes it suitable for such gas sensor applications.⁸ Increasing demand for compact component parts requires miniaturized sensors or semiconductor devices with high structural strength, which can be met with crystalline silicon carbide.⁹

The semiconducting properties of SiC have been used widely for gas sensing applications. The metal-insulator silicon carbide field effect transistor (MISiC-FET) sensor has been shown to be sensitive to NH₃ and also for different combustible gases.¹⁰⁻¹² The electrical properties of Pt/Ga₂O₃/SiC metal oxide semiconductor devices have been used to determine the hydrogen sensing mechanism, which has been achieved by studying the role of the interface states upon the introduction of hydrogen/hydrocarbon (e.g., methane) gases.^{13,14} The MISiC-FET sensor has been tested previously as an NH₃ sensor for selective catalytic reduction systems and has been shown to be sensitive to NH₃ in diesel exhausts.¹⁵ Metal, reactive insulator-based sensors have also

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been developed for hydrocarbon (e.g., methane) sensing with an operational temperature range of 300–600 °C.^{16,17}

Improved SiC piezoresistive pressure sensors have been operated up to 600 °C in both low and high pressure ranges. The sensor response time, which is a critical parameter in feedback process control applications, has been tested for various configurations of catalytic metals used in FET-based sensors.^{18,19} The time constant of the sensors was found to be very small and heavily influenced by temperature. Prototypes of such sensors exhibited a response time less than 10 ms at 500 °C when changing from an oxidizing to a reducing atmosphere.^{20,21} For small power plants (~1 MW), Fourier transform infrared (FTIR) spectroscopy is an expensive technique; so sensors based on electrical response are viable alternatives. SiC-based MISiC-FET sensors, with proper choice of the type and structure of the catalytic gate, can be used for sensing applications. The performance of sensors that are based on the electrical response is affected by the contact lead degradation and the chemical reactions between the metal and semiconductor.²²

In this paper the refractive index of SiC has been analyzed with the change in environmental conditions such as temperature and different gas pressures. A continuous wave helium-neon (He–Ne) laser of wavelength of 632.8 nm is used to probe the changes in the optical property of SiC. The SiC sensor element is inherently a Fabry-Pérot interferometer, enabling optical measurements without any external interferometer.²³ The effects of temperatures and gas pressures on the refractive index of SiC are analyzed using the interference pattern of the laser power reflected by the SiC sensor.

II. EXPERIMENTAL PROCEDURE

A single crystal 4H-SiC wafer of thickness of 399 μm was used as an optical sensor element in this study. The wafer was cleaned by 1 min buffered oxide etching to remove any native oxide from the wafer surface. It was then rinsed in de-ionized (DI) water and soap to remove any dirt. Finally, the organic contaminants were removed from the surface by rinsing the wafer with trichloroethylene, acetone, methanol, and DI water, and then the wafer was dried using a nitrogen gun.

The experimental setup for studying the optical properties of the sensor element is shown in Fig. 1. For high temperature sensing applications, the SiC wafer is placed in a square groove of side of 1 cm on a stainless steel pedestal which is surrounded by a water-cooled copper coil connected to a water-cooled induction heater. The pedestal is heated by the induction heater and the heat is conducted from the pedestal to the wafer. The pedestal also contains a 7.9 mm diameter hole at the center of the groove. This hole beneath the sensor can be filled with different gasses or gas mixtures at high pressures to examine the pressure sensing capability of the sensor. The sensor is held in the groove against the high pressure gasses with a ceramic insulator on top of the wafer, and a copper plate is mounted on the insulator using three copper posts. The insulator and copper plate have a hole at the center to allow the probe (He–Ne laser) beam to reach

FIG. 1. Schematic diagram of the experimental setup for the sensor experiments.

the sensor. The incident laser beam is reflected by the top and bottom surfaces of the SiC wafer, and these reflected beams produce an interference pattern through the mechanism of multibeam interference as in a typical Fabry-Pérot etalon. The interference pattern is calibrated to the temperature of the sensor by measuring its temperature with a thermocouple and recording the interference pattern with a laser power meter using synchronized data acquisition software.

The randomly polarized He–Ne laser beam polarized to transverse electric (TE) mode is normally incident on the sensor after partially transmitting the beam through a beam splitter placed at 45° with respect to the incident beam. After passing through the beam splitter, the beam is incident on the sensor and a fraction of it is reflected back. The reflected beam propagates through the beam splitter again and is received with a detector for measuring the reflected power. Two main sources of error in the power measurement are the vibration of the experimental setup and the resolution of the laser power meter. Various components of the experimental setup were rigidly mounted on an optical table to eliminate any error due to vibrations, and a very high resolution laser power meter capable of measuring power in the range of nanowatts was used. So the error in the experimental results is expected to be less than 1%.

III. EXPERIMENTAL RESULTS AND DISCUSSION

The measured reflected power exhibits a cyclic interference pattern with alternating maximum and minimum powers generated by constructive and destructive interferences of light, respectively.²³ Such patterns are presented in Figs. 2 and 3. A typical cyclic reflected power profile (complementary Airy pattern) with the phase angles (Φ) between the adjacent branches of the reflected power profile has been shown in Fig. 4. A fraction of light that is incident on the

FIG. 2. Reflected power of silicon carbide upon exposure to nitrogen gas at pressures of (a) 100 psi, (b) 200 psi, (c) 300 psi, and (d) 400 psi as a function of temperature from 20 to 300 °C for normal incidence angle.

wafer is transmitted through the wafer. This fraction of light undergoes multiple reflections between the top and the bottom surfaces of the wafer and emerges as phase shifted light, as shown in Fig. 5. This phase shifted light interferes with the small fraction of light that was reflected from the surface of the silicon carbide wafer. The interference between the phase shifted light and the reflected light generates the cyclic interference pattern. The maxima, which correspond to even multiples of the phase angle ϕ , are generated due to constructive interference and minima, which correspond to odd multiples of ϕ , are generated due to destructive interference. These cyclic patterns are also functions of the sensor temperature and pressure.

The cyclic pattern alternates between certain maximum and minimum values with the change in temperature at a constant pressure. These patterns diverge more with the change in temperature at higher pressures. This divergence is unique for the kind of gas or gas mixture used, which indicates that such patterns can be used as a chemical sensor for

different gasses. The effect of various gasses and the effect of temperature and pressure are studied by examining the reflectivity of the silicon carbide wafer.

A. Effect of temperature and pressure on interference

The SiC wafer serves as an amplitude-splitting device, so that two reflected lights may be considered as arising from two coherent virtual sources lying behind the silicon carbide wafer.^{24–26} The reflected lights are parallel on leaving the wafer surface. The optical path length difference between two adjacent reflected beams is given by²⁷ $\Lambda = 2n_{\text{SiC}}d \cos \theta_t$, where Λ is the optical path length, n_{SiC} is the refractive index of the sample, d is the thickness of the sample, and θ_t is the transmitted angle. This expression indicates that a change in the wafer thickness will affect the interference pattern.

The temperature affects the value of d due to the thermal expansion. Typical value of thermal expansion coefficient for silicon carbide is given by²²

FIG. 3. Reflected power of silicon carbide upon exposure to different nitrogen and methane partial gas pressures as a function of temperature from 20 to 350 °C for normal incidence angle: (a) nitrogen 99 psi + methane 1 psi, (b) nitrogen 197 psi + methane 3 psi, (c) nitrogen 296 psi + methane 4 psi, and (d) nitrogen 394 psi + methane 6 psi.

FIG. 4. A typical cyclic reflected power profile (complementary Airy pattern) showing the phase angles (Φ) between the adjacent branches of the cyclic pattern.

$$\alpha(T) = 3.19 \times 10^{-6} + 3.60 \times 10^{-9} \times T - 1.68 \times 10^{-12} T^2. \quad (1)$$

High gas pressures at the interface of the silicon carbide wafer and gas (nitrogen or nitrogen and methane mixture in this study) in Fig. 5 lead to compressive stresses, producing a comparatively denser layer of silicon carbide near its bottom surface. The refractive index of the compressed layer may be different from that of the bulk material. Different gases at the same temperature and pressure can also alter the electron density at the solid-gas interface and thus change the refractive index in a thin layer at the solid surface.

The effect of pressure on the thickness d is taken into account using the expression $d(T_0, P) = d_0(1 - \epsilon)$, where $d(T_0, P)$ is the thickness of the sensor element at room temperature (T_0) and pressure (P). The strain (ϵ) is given by $\epsilon = \sigma/E$, where σ is the applied stress and E is the elastic modulus. The value of elastic modulus has been reported as 392–694 GPa for 4H-SiC.²⁸ In this study an average value of 450 GPa is used for E and the stresses were taken to be 14.7, 100, 200, 300, and 400 psi.

B. Effect of temperature and pressure on phase shift and refractive index

The phase angle is given by²⁷

$$\phi = 2\pi \frac{n(T, P)d(T, P)}{\lambda} \quad (2)$$

for normal incidence of laser beam which is the case in this experiment, where $n(T, P)$ is the refractive index of the

FIG. 5. Schematic diagram for change of optical path length due to pressure.

sample, $d(T, P)$ is the thickness of the sample, and λ is the wavelength of the He-Ne beam. The refractive index of SiC wafer $n(T, P)$ is wavelength dependent due to dispersion effect, temperature dependent due to thermo-optic effect, and pressure dependent due to stress-optic effect.^{29–33} From Eq. (2), the phase shift can be written as

$$\Delta\phi = \frac{2\pi d(T, P)}{\lambda} \Delta n(T, P) + \frac{2\pi n(T, P)}{\lambda} \Delta d(T, P), \quad (3)$$

where $d(T, P) = [1 - (\Delta P/E)]d_0$, $\Delta d(T, P) = d_0\alpha_{\text{mid}}(\Delta T) - (d_0/E)(\Delta P)$, d_0 is the initial thickness of the sample, $\Delta T = T_{m+1} - T_m$, $\Delta P = P_1 - P_0$, P_1 is the pressure at which the sensor response experiment is conducted and P_0 is the initial atmospheric pressure, n_{m+1} and n_m are the refractive indices of silicon carbide at locations l_{m+1} and l_m , i.e., at temperatures T_{m+1} and T_m , respectively, as shown in Fig. 4 and at the pressure P_1 that was applied to the sensor element using nitrogen or nitrogen-methane gas mixture, and E is Young's modulus. In other words, n_m can be written as $n_m = n(T_m, P)$ for a fixed wavelength. Based on Fig. 4, the refractive index of a sample can be obtained from the experimental interference patterns (Figs. 2 and 3) using the following expression:

$$n_{m+1} = \frac{\lambda_0 + n_m d_0 \left[2 - \frac{1}{E}(\Delta P) - \alpha_{\text{mid}}(\Delta T) \right]}{d_0 \left[2 - \frac{3}{E}(\Delta P) + \alpha_{\text{mid}}(\Delta T) \right]}, \quad (4)$$

where α_{mid} is the thermal expansion coefficient of silicon carbide at the temperature corresponding to the midpoint (l_{mid}) of the straight line $l_m l_{m+1}$ in Fig. 4 and can be expressed as $\alpha_{\text{mid}} = \alpha[(T_m + T_{m+1})/2]$.

C. Determination of refractive indices of uncompressed [$n_2(T)$] and compressed [$n_3(T, P)$] layers

Equation (4) can be used to determine the refractive index of the compressed and uncompressed layers of silicon carbide at high temperatures and pressures, if the refractive index of silicon carbide is known at room temperature and atmospheric pressure.

1. Determination of refractive index $n_2(T)$ as a function of temperature

The reflected cyclic interference pattern of SiC is shown in Fig. 6(a) which was obtained by conducting the sensor response experiment under a constant atmospheric pressure (14.7 psi) and temperature ranging from 20 to 375 °C. Substituting $\Delta P = 0$ in Eq. (4), the refractive index [$n_2(T)$] has been determined and plotted in Fig. 6(b). Based on curve fits of the experimental results, the variation of the refractive index with temperature at 14.7 psi gas pressure can be expressed as

$$n_2(T) = 2.31 + 1.66 \times 10^{-3} T + 2.10 \times 10^{-4} T^2 + 4.20 \times 10^{-4} T^3 \quad \text{for } 20 \leq T \leq 375 \text{ } ^\circ\text{C}. \quad (5)$$

FIG. 6. (a) Reflected power of silicon carbide at atmospheric pressure (14.7 psi) and temperature ranging from 20 to 375 °C and (b) comparison of experimental result with the Lorentz-Lorenz model at atmospheric pressure (14.7 psi).

$$r_{23} = \frac{-[(1-R)r_{12} \cos \phi] \pm \sqrt{[(1-R)r_{12} \cos \phi]^2 - (1-Rr_{12}^2)(r_{12}^2 - R)}}{(1-Rr_{12}^2)}, \quad (8)$$

and then the refractive index of the compressed layer n_3 is obtained by the following expression:

$$n_3(T, P) = n_g \frac{1 - r_{23}}{1 + r_{23}}, \quad (9)$$

where n_g is the refractive index of the gas at the wafer-gas interface, and it is related to the gas density by the following Gladstone-Dale relation,³⁴

$$n_g = 1 + R_{GD} \frac{P_1 M}{R^* T}, \quad (10)$$

where R_{GD} is the Gladstone-Dale constant, M is the molecular weight of the gas, R^* is the universal gas constant, T is the absolute temperature, and P_1 is the total pressure of the gas. The values of R_{GD} are 0.238 and 0.653 cm³/g for nitrogen and methane, respectively.³⁴ The Gladstone-Dale constant for gas mixtures can be expressed as $R_{GD} = \sum R_{GD_i} x_i$, where R_{GD_i} and x_i are the Gladstone-Dale constant and mole fraction for the i th species in the mixture, respectively.

2. Determination of refractive index $n_3(T, P)$ as a function of temperature and pressure from the experimental data using a three-layer model for interference due to multiple reflections

A three-layer model has been used to obtain the refractive index of silicon carbide from the reflectivity data for different gas pressures. In this model, the reflection of the He-Ne beam is considered to be affected by three layers, as shown in Fig. 5. The three layers can be identified as layer 1 which is the ambient air at the top surface of the silicon carbide wafer, layer 2 which is the uncompressed portion of the original silicon carbide wafer, and layer 3 which is the compressed layer formed due to the pressure of the gas beneath the wafer. The reflectance R of these three layers can be expressed as²⁷

$$R = \frac{r_{12}^2 + r_{23}^2 + 2r_{12}r_{23} \cos \phi}{1 + r_{12}^2 r_{23}^2 + 2r_{12}r_{23} \cos \phi}, \quad (6)$$

where r_{12} and r_{23} are Fresnel reflection coefficients of the interfaces between layers 1 and 2, and layers 2 and 3, respectively. r_{12} is determined using Fresnel's relation

$$r_{12} = \frac{n_2(T) - 1}{n_2(T) + 1}, \quad (7)$$

where n_2 , which is the refractive index of the uncompressed layer of SiC sample, is obtained as a function of only temperature from Eq. (5). Equation (6) can be solved for r_{23} , i.e.,

Based on Eq. (10), Eq. (9) can be rewritten to express n_3 as a function of temperature and pressure as follows:

$$n_3(T, P) = \left(1 + R_{GD} \frac{P_1 M}{R^* T}\right) \frac{1 - r_{23}}{1 + r_{23}}. \quad (11)$$

The reflectance data are used to calculate r_{23} using Eq. (8). The value of ϕ at any point on the observed interference pattern is obtained through linear interpolation along each arm of the pattern and by noting that the maximum and minimum points in the pattern correspond to even and odd multiples of π , respectively. The refractive index of the compressed layer has been determined using Eq. (11) and presented in Figs. 7 and 8.

D. Analysis of temperature- and pressure-dependent refractive index based on Lorentz-Lorenz model

The experimental data for the variation of refractive index with temperature at 1 atm pressure are compared with theoretical results based on Lorentz-Lorenz model in Fig. 6.

FIG. 7. (a). Refractive index of the compressed layer upon exposure to 100 psi nitrogen pressure as a function of temperature from 20 to 400 °C. (b). Refractive index of the compressed layer upon exposure to 200 psi nitrogen pressure as a function of temperature from 20 to 400 °C. (c). Refractive index of the compressed layer upon exposure to 300 psi nitrogen pressure as a function of temperature from 20 to 400 °C. (d). Refractive index of the compressed layer upon exposure to 400 psi nitrogen pressure as a function of temperature from 20 to 400 °C.

Considering bound and free electrons in semiconductors, the multioscillator model^{34–37} provides the following expression for the refraction index:

$$n^2 = 1 + \sum_{j=1}^{p'} \frac{N_1 e^2}{\epsilon_0 m} \frac{f_j}{\omega_{0j}^2 - \omega^2}, \quad (12)$$

bound

where N_1 is the valance electron concentration, e is the electronic charge, ϵ_0 is the permittivity of vacuum, m is the effective mass, f_j is the strength of the j th Lorentz oscillator, ω_{0j} is the resonant frequency of the j th Lorentz oscillator, and ω is the frequency of the incident laser beam. Equation (12) can be simplified to the following form for a single oscillator model.^{34,35}

$$n^2 = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2}. \quad (13)$$

Here ω_p is the electronic plasma frequency given by $\omega_p = \sqrt{Ne^2/(\epsilon_0 m)}$, where N is the number of electrons per unit volume, e is the electronic charge, ϵ_0 is the permittivity of

free space, and m is the mass of an electron. ω_0 is an average resonant frequency, which is estimated by considering $\hbar\omega_0$ to be equal to the band gap energy E_g , where $\hbar$ is the Planck constant. Both N and E_g depend on the temperature and pressure. Since N depends on the volume of the material and the volume expands as the temperature increases and contracts as the pressure increases, an expression for N can be obtained due to these two effects, and then the plasma frequency can be written as

$$\omega_p^2 = \frac{e^2 N_0}{\epsilon_0 m \left[1 + 3\alpha\Delta T - \frac{\Delta P}{E} (1 + 2\alpha\Delta T) \right]}, \quad (14)$$

where N_0 is the electron density of the sample based on the initial volume at the initial pressure (P_0) and temperature (T_0).

Considering that the band gap energy $E_g(T, P)$ depends on the temperature and pressure linearly,³⁸ the following expression can be written for the average resonant frequency:

FIG. 8. (a). Refractive index of the compressed layer upon exposure to nitrogen and methane partial (nitrogen 99 psi+methane 1 psi) pressures as a function of temperature from 20 to 400 °C. (b) Refractive index of the compressed layer upon exposure to nitrogen and methane partial (nitrogen 197 psi +methane 3 psi) pressures as a function of temperature from 20 to 400 °C. (c). Refractive index of the compressed layer upon exposure to nitrogen and methane partial (nitrogen 296 psi+methane 4 psi) pressures as a function of temperature from 20 to 400 °C. (d). Refractive index of the compressed layer upon exposure to nitrogen and methane partial nitrogen 394 psi+methane 6 psi) pressures as a function of temperature from 20 to 400 °C.

$$\omega_0 = \frac{2\pi}{h} E_g(T, P) = \frac{2\pi}{h} \left[E_g(0) + \frac{\partial E_g}{\partial T} \Delta T + \frac{\partial E_g}{\partial P} \Delta P \right], \quad (15)$$

where $\partial E_g / \partial T$ and $\partial E_g / \partial P$ are the temperature and pressure coefficients, respectively. The value of $\partial E_g / \partial T$ has been

reported³⁶ to be -3.3×10^{-4} eV/K and the value of $\partial E_g / \partial P$ has been reported³³ to be 0.21 eV/Mbar.

Applying expressions ω_p and ω_0 into Eq. (13) and letting $n=n_3$, the following expression is obtained for the refractive index of the compressed layer:

$$n_3^2 = 1 + \frac{e^2 N_0}{\epsilon_0 m \left[1 + 3\alpha \Delta T - \frac{\Delta P}{E} (1 + 2\alpha \Delta T) \right] \left\{ \left(\frac{2\pi}{h} \right)^2 \left[E_g(0) + \frac{\partial E_g}{\partial T} \Delta T + \frac{\partial E_g}{\partial P} \Delta P \right]^2 - \omega_L^2 \right\}}, \quad (16)$$

where ω_L is the angular frequency of the laser used for probing the sensor response. This theoretical value of n_3 is compared to the experimental data in Figs. 6–8. Eliminating n_3

from Eq. (16) using Eq. (11), the gas pressure can be determined from the following expression by knowing the gas temperature:

FIG. 9. Laser-microstructured embedded SiC layer acting as an optical absorber to produce an optical response as a function of temperature only, i.e., the embedded layer acts as an uncompressed layer because it is not affected by the gas pressure, making the embedded SiC layer a suitable temperature sensor.

$$A_5 \left(\frac{P_1 - P_0}{E} \right)^5 + A_4 \left(\frac{P_1 - P_0}{E} \right)^4 + A_3 \left(\frac{P_1 - P_0}{E} \right)^3 + A_2 \left(\frac{P_1 - P_0}{E} \right)^2 + A_1 \left(\frac{P_1 - P_0}{E} \right) + A_0 = 0, \quad (17)$$

where A_5 , A_4 , A_3 , A_2 , A_1 , and A_0 are constants as defined in Appendix A.

E. Sensor response decoupling model for determining the temperature and pressure

In practical sensor applications, the measured data will be only the reflectance R . To determine the temperature and pressure based on R , the values of $n_2(T)$, $n_3(T, P)$, and ϕ must be known. We have developed the following four-step model to determine the temperature based on the reflectance from two regions of the silicon carbide sensor. One of the regions contains an embedded optical absorber produced by a laser-microstructuring technique and the other region is the original silicon carbide.

1. Step 1: Determination of temperature using an optical absorber in SiC

The cyclic interference patterns in Figs. 2 and 3 are multivalued functions of temperature and pressure, which cannot be used directly to measure temperature and pressure. A monotonic optical response of SiC with respect to temperature will allow determination of temperature uniquely. To achieve such response, an optical absorber was created using a laser-embedded microstructuring technique.^{39,40} The optical absorber was produced inside the SiC wafer as shown in Fig. 9 with a high intensity Nd:YAG (yttrium aluminum garnet) pulsed laser beam (average laser power=8.5 W, pulse repetition rate=5 kHz, beam radius at the surface of the sample=50.5–55 μm with the laser focal spot being 5 mm

FIG. 10. Monotonic optical response of laser-microstructured embedded SiC temperature sensor used for decoupling the temperature and pressure when a SiC crystal is used as a sensor.

above the top surface of the sample, laser beam scanning speed=1 mm/s) in the presence of methane gas at 30 psi pressure.

The optical response²⁶ of the absorber was obtained as a function of temperature for the He–Ne laser as presented in Fig. 10, which shows that the cyclic variation in the reflected power is negligibly small compared to that observed in Figs. 2 and 3. The reflected power in Fig. 10 can be considered as a monotonic function of temperature, and this characteristic makes the sample a potential temperature sensor.

Since the reflected power (P_r) represents the sensor response above the optical absorber without any reflection from the wafer-gas interface at the bottom surface of the sensor, there is no pressure effect in the reflected data. Using these data, the Fresnel reflection coefficient of the interface of layers 1 and 2 can be determined as $r_{12}=P_r/P_i$, where P_i is the incident He–Ne laser power on the surface of the SiC sensor. Now Eq. (7) can be used to determine $n_2(T)$ using the value of r_{12} , and then the temperature can be determined knowing $n_2(T)$ as a function of T , as shown in Eq. (5).

2. Step 2: Determination of the Fresnel reflection coefficient r_{23}

The reflected power from the second region of the sensor represents a single point on the cyclic interference pattern shown in Figs. 2 and 3. The reflectance R can be calculated based on the observed reflected power and the incident laser power, and then the Fresnel reflection coefficient r_{23} is obtained from Eq. (8). The phase change ϕ in Eq. (8) is taken as $\phi=\phi_r$, as derived in Appendix B.

3. Step 3: Determination of pressure

Method 1. The pressure P can be determined from Eq. (17) by evaluating the coefficients A_i , $i=0,1,2,\dots,5$ based on various properties of the sensor material and the temperature obtained in step 1. Since Eq. (17) is a fifth order polynomial, it will yield five roots with three distinct possibilities: (i) one real root and four complex roots, (ii) one positive root and four negative roots, and (iii) more than one positive root. While the real root in case (i) and the single positive root in case (ii) can be selected as the gas pressure, care must

FIG. 11. (a). Refractive index of the compressed layer upon exposure to different temperatures as a function of nitrogen pressure (Y axis in $\ln$ scale). (b). Refractive index of the compressed layer upon exposure to different temperatures as a function of nitrogen and methane partial pressures (Y axis in $\ln$ scale).

be taken to select the appropriate pressure in case (iii).

Method 2: Differential model (our model) developed in this study. Considering that n_3 varies with temperature and pressure linearly, it can be expressed as

$$\Delta n_3(T, P) = \frac{\partial n_3}{\partial T} \Delta T + \frac{\partial n_3}{\partial P} \Delta P, \quad (18)$$

which can be rewritten as

$$n_3(T_1, P_1) - n_3(T_0, P_0) = \frac{\partial n_3}{\partial T} (T_1 - T_0) + \frac{\partial n_3}{\partial P} (P_1 - P_0), \quad (19)$$

where $n_3(T_0, P_0)$ is the refractive index at room temperature (T_0) and one atmospheric pressure (P_0); $n_3(T_1, P_1)$ can be obtained from step 3. The normalized thermo-optic coefficients $[1/n_3(\partial n_3/\partial T)]$, have been obtained from the experimental data in Figs. 7 and 8 by approximating the curves as two linear segments in the temperatures ranges of 20–100 and 100–400 °C and then determining the slopes of each

TABLE I. Experimental values of $(1/n_3)(\partial n_3/\partial T)$ at different pressures.

Pressure (psi)	Values of $(1/n_3)(\partial n_3/\partial T)$ ($^{\circ}\text{C}^{-1}$)			
	Pure N_2		Mixture of N_2 and CH_4 gases	
	20–100 °C	100–400 °C	20–100 °C	100–400 °C
100	-0.62×10^{-5}	0	-0.23×10^{-3}	0
200	-3.7×10^{-5}	-1.73×10^{-5}	-1.97×10^{-3}	-1.57×10^{-3}
300	-6.2×10^{-5}	-1.73×10^{-5}	-1.45×10^{-3}	-1.57×10^{-3}
400	-7.12×10^{-5}	-1.73×10^{-5}	-1.31×10^{-3}	-1.57×10^{-3}

segment. The normalized stress-optic coefficients $[1/n_3(\partial n_3/\partial P)]$ have been obtained from the experimental data in Figs. 11(a) and 11(b) by calculating the slopes of the linear segments in the pressure ranges of 20–100 and 100–400 psi. It can be observed in Figs. 11(a) and 11(b) that the slopes are significantly different up to the gas pressure of 100 psi, but it is almost the same at higher pressures for both pure nitrogen and nitrogen-methane mixture. The values of these coefficients are tabulated in Tables I and II. A single value of the normalized stress-optic coefficient can be used for high pressure sensing applications. Knowing T_1 from step 1 and n_3 from step 3, the gas pressure P_1 can be obtained from Eq. (17).

IV. COMPARISON OF THEORETICAL MODELS WITH EXPERIMENTAL DATA

The refractive index of the compressed layer (n_3) has been calculated as a function of temperature (20–400 °C) for four different pressures (50, 100, 300, and 400 psi) using two theoretical models (Lorentz-Lorenz model [Eq. (16) and differential model Eq. (19)]. n_3 has also been obtained from the experimental data (interference patterns in Figs. 2 and 3) using Eq. (3) and compared with the model results in Figs. 7(a)–7(d). Although the Lorentz-Lorenz model compares well with the experimental data at 50 psi, it differs significantly at higher pressures (100, 300, and 400 psi), as shown in Figs. 7(b)–7(d). This discrepancy may be because the calculation of the electron density (N) and the linear variation of the band gap (E_g) energy with respect to temperature and pressure in the Lorentz-Lorenz model are good approximations at low pressures. Additionally the Lorentz-Lorenz model requires the values of different physical properties, such as the effective masses and deformation potentials at the X point of the Brillouin zone, which are unknown.

TABLE II. Experimental values of $(1/n_3)(\partial n_3/\partial P)$ at different temperatures.

Temperature ($^{\circ}\text{C}$)	Values of $(1/n_3)(\partial n_3/\partial P)$ (psi^{-1})			
	Pure N_2		Mixture of N_2 and CH_4 gases	
	20–100 psi	100–400 psi	20–100 psi	100–400 psi
20	-1.8×10^{-4}	-3.2×10^{-4}	-3.4×10^{-4}	-5.4×10^{-4}
100	-1.9×10^{-4}	-3.2×10^{-4}	-4.5×10^{-4}	-5.4×10^{-4}
200	-3.0×10^{-3}	-3.2×10^{-4}	-2.8×10^{-3}	-5.4×10^{-4}
300	-5.7×10^{-3}	-3.2×10^{-4}	-5.5×10^{-3}	-5.4×10^{-4}
400	-11.6×10^{-3}	-3.2×10^{-4}	-12.1×10^{-3}	-5.4×10^{-4}

The refractive index (n_3) obtained from the differential model of this study compares well with the experimental data over the entire temperature and pressure ranges investigated in this study. This model, therefore, can be used to analyze the optical response of SiC for pressure measurement. The model results also compare well with the experimental data for two different gases, pure nitrogen, and a nitrogen-methane mixture as, shown in Figs. 8(a)–8(d), indicating the potential of this model for identifying the chemical species based on the optical response of the SiC sensor. The Lorentz-Lorenz model [Eq. (16)] cannot, however, distinguish the effect of different kinds of gases because only the total pressure and not the electronic interaction of different gases with SiC is considered while deriving Eq. (16).

V. CONCLUSION

The effects of a single gas and a gas mixture on the optical properties of 4H-SiC have been studied as a function of temperature and pressure. The reflected power of the wafer exhibited unique interference patterns for both nitrogen and nitrogen-methane gas mixture at high pressures and temperatures. The width of the pattern tends to increase with the increase in the gas pressure. These patterns can be utilized to determine the refractive indices of SiC and to identify the underlying gas.

APPENDIX A

Expressions for various constants that appear in Eq. (17).

$$A_5 = \left(R_{GD} \frac{EM}{R^*T} \right)^2 \left(\frac{1-r_{23}}{1+r_{23}} \right)^2 (1+2\alpha\Delta T)(1+3\alpha\Delta T) \frac{E}{E_g(0)} \frac{\partial E_g}{\partial P},$$

$$A_4 = \left(\frac{1-r_{23}}{1+r_{23}} \right) \frac{E}{E_g(0)} \frac{\partial E_g}{\partial P} \left[\left(R_{GD} \frac{EM}{R^*T} \right)^2 (1+3\alpha\Delta T) - 2 \right] - \left(R_{GD} \frac{EM}{R^*T} \right)^2 (1+2\alpha\Delta T) \left[1 + \frac{1}{E_g(0)} \frac{\partial E_g}{\partial T} \Delta T \right] \\ - 2 \left(1 + R_{GD} \frac{P_0 M}{R^*T} \right) \left(R_{GD} \frac{EM}{R^*T} \right) (1+2\alpha\Delta T)(1+3\alpha\Delta T),$$

$$A_3 = 2 \left(1 + R_{GD} \frac{P_0 M}{R^*T} \right) \left(R_{GD} \frac{EM}{R^*T} \right) \left(\frac{1-r_{23}}{1+r_{23}} \right)^2 (1+3\alpha\Delta T) \frac{E}{E_g(0)} \frac{\partial E_g}{\partial P} - \left[\left(1 + R_{GD} \frac{P_0 M}{R^*T} \right) \left(\frac{1-r_{23}}{1+r_{23}} \right)^2 - 1 \right] \\ \times (1+2\alpha\Delta T)(1+3\alpha\Delta T) \frac{E}{E_g(0)} \frac{\partial E_g}{\partial P} - 4 \left(1 + R_{GD} \frac{P_0 M}{R^*T} \right) \left(R_{GD} \frac{EM}{R^*T} \right) \left(\frac{1-r_{23}}{1+r_{23}} \right)^2 (1+2\alpha\Delta T) \\ \times \left[1 + \frac{1}{E_g(0)} \frac{\partial E_g}{\partial T} \Delta T \right] \frac{E}{E_g(0)} \frac{\partial E_g}{\partial P} + 2 \left(R_{GD} \frac{EM}{R^*T} \right)^2 \left(\frac{1-r_{23}}{1+r_{23}} \right)^2 (1+3\alpha\Delta T) \frac{E}{E_g(0)} \frac{\partial E_g}{\partial P} \left[1 + \frac{1}{E_g(0)} \frac{\partial E_g}{\partial T} \Delta T \right] \\ - \left(R_{GD} \frac{EM}{R^*T} \right)^2 \left(\frac{1-r_{23}}{1+r_{23}} \right)^2 (1+2\alpha\Delta T) \left[1 + \frac{1}{E_g(0)} \frac{\partial E_g}{\partial T} \Delta T \right]^2,$$

The refractive index data can be used in mathematical models to measure the temperature and pressure of different gases. A laser-microstructured SiC temperature sensor exhibits monotonic change in the reflected power as a function of temperature, indicating that the sensor is suitable for temperature measurement. Optical response from the nonmicrostructured section of the sensor contains the effects of both the temperature and pressure. A mathematical model has been presented to decouple the effect of pressure so that the sensor can be used to measure the gas pressure as well.

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$$\begin{aligned}
A_2 = & \left[\left(1 + R_{\text{GD}} \frac{P_0 M}{R^* T} \right)^2 \left(\frac{1 - r_{23}}{1 + r_{23}} \right)^2 - 1 \right] (1 + 3\alpha \Delta T) \frac{E}{E_g(0)} \frac{\partial E_g}{\partial P} - 2 \left[\left(1 + R_{\text{GD}} \frac{P_0 M}{R^* T} \right)^2 \left(\frac{1 - r_{23}}{1 + r_{23}} \right)^2 - 1 \right] \\
& \times (1 + 2\alpha \Delta T) \left[1 + \frac{1}{E_g(0)} \frac{\partial E_g}{\partial T} \Delta T \right] \frac{E}{E_g(0)} \frac{\partial E_g}{\partial P} + 4 \left(1 + R_{\text{GD}} \frac{P_0 M}{R^* T} \right) \left[1 + \frac{1}{E_g(0)} \frac{\partial E_g}{\partial T} \Delta T \right] \left(\frac{1 - r_{23}}{1 + r_{23}} \right)^2 (1 + 3\alpha \Delta T) \frac{E}{E_g(0)} \frac{\partial E_g}{\partial P} \\
& \times \left[1 + \frac{1}{E_g(0)} \frac{\partial E_g}{\partial T} \Delta T \right] - 2 \left(1 + R_{\text{GD}} \frac{P_0 M}{R^* T} \right) \left(R_{\text{GD}} \frac{EM}{R^* T} \right) \left(\frac{1 - r_{23}}{1 + r_{23}} \right)^2 \left\{ (1 + 2\alpha \Delta T) \left[1 + \frac{1}{E_g(0)} \frac{\partial E_g}{\partial T} \Delta T \right] \frac{E}{E_g(0)} \frac{\partial E_g}{\partial P} \right\} \\
& - 2 \left(1 + R_{\text{GD}} \frac{P_0 M}{R^* T} \right) \left(R_{\text{GD}} \frac{EM}{R^* T} \right) \left(\frac{1 - r_{23}}{1 + r_{23}} \right)^2 (1 + 2\alpha \Delta T) \left[1 + \frac{1}{E_g(0)} \frac{\partial E_g}{\partial T} \Delta T \right]^2 \\
& + \left\{ (1 + 3\alpha \Delta T) \left[1 + \frac{1}{E_g(0)} \frac{\partial E_g}{\partial T} \Delta T \right]^2 - \left[\frac{h\omega_L}{2\pi E_g(0)} \right]^2 \right\} \left(R_{\text{GD}} \frac{EM}{R^* T} \right)^2 \left(\frac{1 - r_{23}}{1 + r_{23}} \right)^2, \\
A_1 = & 2 \left[\left(1 + R_{\text{GD}} \frac{P_0 M}{R^* T} \right)^2 \left(\frac{1 - r_{23}}{1 + r_{23}} \right)^2 - 1 \right] \left[1 + \frac{1}{E_g(0)} \frac{\partial E_g}{\partial T} \Delta T \right] \frac{E}{E_g(0)} \frac{\partial E_g}{\partial P} - \left(1 + R_{\text{GD}} \frac{P_0 M}{R^* T} \right)^2 \left(\frac{1 - r_{23}}{1 + r_{23}} \right)^2 \\
& - (1 + 2\alpha \Delta T) \left[1 + \frac{1}{E_g(0)} \frac{\partial E_g}{\partial T} \Delta T \right]^2 + 2 \left\{ (1 + 3\alpha \Delta T) \left[1 + \frac{1}{E_g(0)} \frac{\partial E_g}{\partial T} \Delta T \right]^2 - \left[\frac{h\omega_L}{2\pi E_g(0)} \right]^2 \right\} \\
& \times \left(1 + R_{\text{GD}} \frac{P_0 M}{R^* T} \right) \left(R_{\text{GD}} \frac{EM}{R^* T} \right) \left(\frac{1 - r_{23}}{1 + r_{23}} \right)^2, \\
A_0 = & \left[\left(1 + R_{\text{GD}} \frac{P_0 M}{R^* T} \right)^2 \left(\frac{1 - r_{23}}{1 + r_{23}} \right)^2 - 1 \right] \left\{ (1 + 3\alpha \Delta T) \left[1 + \frac{1}{E_g(0)} \frac{\partial E_g}{\partial T} \Delta T \right]^2 - \left[\frac{h\omega_L}{2\pi E_g(0)} \right]^2 \right\} - \frac{e^2 N_0}{\epsilon_0 m} \left(\frac{h}{2\pi E_g(0)} \right)^2.
\end{aligned}$$

APPENDIX B

The phase shift ϕ is given by $\phi = 2\pi[n(T, P)d(T, P)/\lambda]$ as in Eq. (2). Let ϕ_u and ϕ_c be the phase shifts due to the passage of He–Ne laser beam through the uncompressed (no pressure effect) and compressed layers, respectively. The total phase shift ϕ_t can be expressed as

$$\begin{aligned}
\phi_t = \phi_u + \phi_c &= \frac{2\pi}{\lambda} [n_2(T)(d - d_c) + n_3(T, P)d_c] \\
&= \frac{2\pi}{\lambda} \{n_2(T)d + [n_3(T, P) - n_2(T)]d_c\},
\end{aligned}$$

where d is the total thickness of the SiC sensor and d_c is the thickness of the compressed layer. The compressed layer is generally very thin compared to the thickness of the sensor and the difference in the refractive index, i.e., $n_3(T, P) - n_2(T)$ is expected to be much less than the value of $n_2(T)$. So ϕ_t can be written as

$$\phi_t \approx 2\pi \frac{n_2(T)d}{\lambda},$$

and the value of $n_2(T)$ can be obtained from step 1 in Sec. III E. This expression of ϕ_t is substituted for ϕ in Eq. (8) while determining the Fresnel reflection coefficient r_{23} in step 2 in Sec. III E.

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