

Postprocessing lattice strain in 4H-SiC

Helton Goncalves de Medeiros^{1,*} Agatha Christie Ulibarri^{1,2} Piyush Kumar,¹ Maria Mendes Martins,^{1,3}
Marianne Etzelmüller Bathen^{1,4} and Ulrike Grossner¹

¹Advanced Power Semiconductor Laboratory, *ETH Zürich*, Physikstrasse 3, 8092 Zürich, Switzerland

²University of Melbourne, School of Physics, Parkville, Victoria, Australia

³PSI Center for Neutron and Muon Sciences, 5232 Viligen PSI, Switzerland

⁴Department of Physics/Centre for Materials Science and Nanotechnology,
University of Oslo, 0316 Oslo, Norway



(Received 3 November 2025; revised 22 February 2026; accepted 18 June 2026; published 20 July 2026)

Processing steps, such as thermal oxidation, creation of p- and n-doped regions via ion implantation, and postoxidation and postimplantation annealing, are essential for successful and reliable fabrication of devices based on 4H-SiC. These processing steps are known to introduce crystalline defects or even modifications within the SiC base material that can potentially compromise device operation and reliability. In this work, we systematically study the strain introduced in the 4H-SiC crystal by SiC-specific manufacturing methods. The results show that tensile strain is present after ion implantation, thermal oxidation, and subsequent annealing processes. Interestingly, aluminum implanted samples show compressive strain near the surface in addition to the presence of an additional Raman signature, while nitrogen and phosphorus implanted samples experience tensile strain. Density functional theory calculations were performed to corroborate the experimental data and connect the type of strain to the microscopic impact that different dopants have on the SiC lattice. These results contribute to the understanding of processing-induced modifications within the crystal and show that Raman spectroscopy is a powerful tool to assess modifications to the 4H-SiC crystal.

DOI: [10.1103/tmj1-xzgr](https://doi.org/10.1103/tmj1-xzgr)

I. INTRODUCTION

Silicon carbide (SiC) is a wide bandgap semiconductor that is well established in power electronics applications as an alternative to silicon (Si) technologies. Moreover, SiC is an attractive material for a wide range of applications—including quantum technology, automotive, and aerospace—due to its high operating temperature and low on-state power losses [1–3]. However, defects and material modifications caused by SiC-specific wafer and device manufacturing processes continue to pose challenges, especially for ruggedness, robustness, and long-term reliability [4]. SiC device fabrication uses techniques similar to well-established Si technologies, including metal deposition and thermal oxidation, while ion implantation doping and subsequent thermal treatment require adjustments to process parameters and dedicated equipment.

Thermal oxidation leads to the creation of defects in the 4H-SiC epitaxial layer, at the oxide/SiC interface, and within the oxide layer itself [5–8]. Those defects impact the electrical performance of metal-oxide-semiconductor field-effect transistors (MOSFETs) [9,10]. To improve the electrical performance, postoxidation annealing (POA) is implemented to reduce the density of interface defects and increase channel mobility [6]. In addition to reducing the population of interface defects, the POA process in a nitric oxide (NO) environment introduces a high concentration of nitrogen near the surface [11] and bulk defects within the epitaxial layer [5]. Apart from electrically active defects, thermal oxidation also creates optically active defects and induces strain in the crystal [12].

Ion implantation is the process of choice for creating n- and p-type regions in 4H-SiC due to the low diffusivity of elements in the host crystal [13]. Typical dopants are nitrogen (N) and phosphorus (P) for n-type doping and aluminum (Al) for p-type doping. After ion implantation, a postimplantation annealing (PIA) step is performed to activate the dopants and to reduce the ion-induced crystal damage [14]. However, intrinsic and extrinsic defects are known to still be present after ion implantation and the PIA process [15].

*Contact author: medeiros@aps.ee.ethz.ch

Published by the American Physical Society under the terms of the [Creative Commons Attribution 4.0 International](https://creativecommons.org/licenses/by/4.0/) license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

Lattice strain in a semiconductor crystal can be measured using Raman spectroscopy, a nondestructive technique requiring minimal sample preparation [16]. This strain may originate from residual stress due to epitaxial growth [17], or it may be induced by processing steps such as thermal oxidation [12], ion implantation with post-implantation anneal (PIA) [18], or the packaging process [19]. In Si integrated circuits, Raman spectroscopy has been extensively used to evaluate strain [20]. The strain within the crystal changes the SiC properties, resulting in variations in the emission of the color centers as used in quantum technologies, shown for 6H-SiC [21], and altering the expansion of stacking faults, which are related to bipolar degradation in SiC power devices [22].

This work studies the strain induced by key SiC processing steps, including thermal oxidation followed by different POA conditions, ion implantation with N, P, and Al dopants, and also considers the influence of PIA and thermal treatments. We aim to understand the state of modification in the 4H-SiC crystal by means of Raman spectroscopy measurements with supporting interpretation by density functional theory (DFT) calculations.

II. METHODOLOGY

A. Sample description

A series of samples with different epitaxial (epi) layer thicknesses (10 and 30 μm), doping concentrations (2×10^{15} , 4×10^{15} , and $1 \times 10^{17} \text{ cm}^{-3}$), and doping types (n- and p-type) were used as pristine samples, as described in Table I. All epitaxial layers are 4° off axis [0001] 4H-SiC wafers, thus all processing steps described were performed on the Si-face. For the ion implantation, samples with 10 μm -thick epilayers and an n-type doping concentration of $4 \times 10^{15} \text{ cm}^{-3}$ were used. These samples were implanted with either N, P, or Al at different concentrations, see Table II for further details. For the N- and P-implanted samples, a 300 nm box profile was created for two resulting doping concentrations (1×10^{17} and $1 \times 10^{18} \text{ cm}^{-3}$), which means that several implantation steps at different energies were used. The PIA for the N- and P-ion-implanted samples was performed for 30 min at 1600 $^\circ\text{C}$. In contrast, the Al-implanted samples were

TABLE I. Description of the pristine samples, including the sample identifier, thickness of the epitaxial layer, doping concentration ($N_{D,A}$), and dopant.

Sample ID	Epi thickness (μm)	$N_{D,A} (\text{cm}^{-3})$	Dopant
Epi _{10 μm} -N ₁₅	10	4×10^{15}	Nitrogen
Epi _{10 μm} -N ₁₇	10	1×10^{17}	Nitrogen
Epi _{10 μm} -Al ₁₇	10	1×10^{17}	Aluminum
Epi _{30 μm} -N ₁₅	30	2×10^{15}	Nitrogen

exposed to a single energy Al implantation, where the implantation fluence was adjusted to obtain implantation concentrations of 1×10^{18} and $1 \times 10^{20} \text{ cm}^{-3}$ within the first 100 nm. For the Al-implanted samples, samples both with and without PIA were investigated. The PIA for the Al samples was conducted for 30 min at 1700 $^\circ\text{C}$. For more details about the Al samples see Ref. [23]. All PIA thermal treatments were performed with a carbon cap to prevent the out-diffusion of Si during annealing.

For the thermally oxidized sample set, the epilayer thickness was 30 μm with n-type doping concentration of $2 \times 10^{15} \text{ cm}^{-3}$. All the samples were thermally oxidized at 1300 $^\circ\text{C}$ for approximately equal to 30 min, as described in Table III. Sample Epi_{30 μm} -N₁₅-Ar1300 was only annealed in an Ar environment at 1300 $^\circ\text{C}$ as a reference sample. The studied samples were exposed to similar thermal oxidation but differ in the postoxidation annealing (POA) treatment. For more details about the samples, see Ref. [11].

B. Raman spectroscopy

The Raman measurements were performed with a LabRAM HR Evolution UV-VIS-NIR from Horiba. The

TABLE II. Description of the ion-implanted samples, including the sample identifier, ion type, doping concentration ($N_{D,A}$), and PIA conditions. For all samples, the epilayer thickness is 10 μm and the doping type is n-type with $4 \times 10^{15} \text{ cm}^{-3}$ free carrier concentration.

Sample ID	Ion	$N_{D,A} (\text{cm}^{-3})$	PIA
Imp-N ₁₇ -PIA	N	1×10^{17}	30 min at 1600 $^\circ\text{C}$
Imp-N ₁₈ -PIA	N	1×10^{18}	
Imp-P ₁₇ -PIA	P	1×10^{17}	30 min at 1600 $^\circ\text{C}$
Imp-P ₁₈ -PIA	P	1×10^{18}	
Imp-Al ₁₈	Al	1×10^{18}	No PIA
Imp-Al ₂₀	Al	1×10^{20}	
Imp-Al ₁₈ -PIA	Al	1×10^{18}	30 min at 1700 $^\circ\text{C}$
Imp-Al ₂₀ -PIA	Al	1×10^{20}	

TABLE III. Description of the thermally oxidized samples, including the sample identifier, thermal oxidation condition, and POA treatment. For all samples, the epi thickness is 30 μm and the doping type is n-type with $2 \times 10^{15} \text{ cm}^{-3}$ concentration. The POA process took 70 min.

Sample ID	Thermal oxidation	POA
1300 $\times$	32 min at 1300 $^\circ\text{C}$	Not applicable
1300NO1150	30 min at 1300 $^\circ\text{C}$	NO at 1150 $^\circ\text{C}$
1300NO1300	28 min at 1300 $^\circ\text{C}$	NO at 1300 $^\circ\text{C}$
1300Ar1300	32 min at 1300 $^\circ\text{C}$	Ar at 1300 $^\circ\text{C}$
Epi _{30 μm} -N ₁₅ -Ar1300	30 min in Ar at 1300 $^\circ\text{C}$	Not applicable

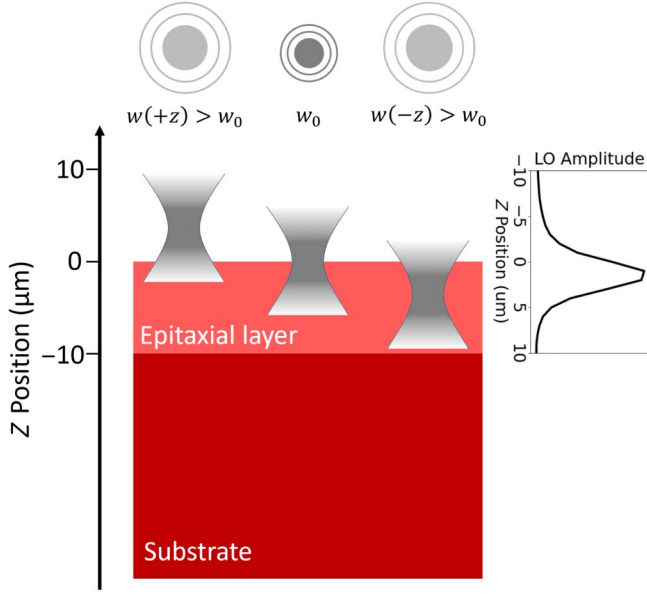


FIG. 1. Schematic of the beam waist and DOF characterization for the Epi_{10 μm}-N₁₅ sample.

excitation wavelength was 532 nm and all the measurements were recorded at room temperature. To ensure adequate spectral resolution, a grating of 1800 gr/mm was employed. Spectrometers are known to have thermal fluctuations [24,25], which change the peak position of the Raman spectra. To account for the fluctuations, three points were measured at the surface for each sample, and the error bar is presented. In addition, to enable comparison between strain measurements taken on different days, the reference spectrum was always collected with the same calibration settings as the samples of interest.

The Raman spectra from different probing depths and volumes were accessed by using 50× and 100× magnification objectives. The Gaussian beam depth of focus (DOF) and beam waist (w_0) were experimentally measured on the Epi_{10 μm}-N₁₅ sample in the following way. Images of the beam were taken at depths (Z positions) varying from -10 to 10 μm, where the 0 μm point was assigned to the sample surface, as illustrated in Fig. 1. The z movement was performed by a piezoelectric stage with a precision of 1 nm. The full width at half maximum (FWHM) of the beam was measured for distinct depths. The minimum FWHM, measured at the sample surface, was determined to be the beam waist. The DOF was evaluated by recording the Raman spectra from -10 to 10 μm and evaluating the Lorentzian amplitude profile of the 996 cm^{-1} longitudinal optical plasmon coupled (LOPC) mode. The 996 cm^{-1} LOPC signature was selected for the DOF evaluation because it is sensitive to doping concentration [26] and therefore gives a different spectral signature for the epilayer and substrate regions. The inset in Fig. 1 shows the rise and decay of the LO amplitude. By taking the

TABLE IV. Measured Gaussian beam parameters, laser power at the sample, and the power density.

	50× (NA: 0.5)	100× (NA: 0.9)
Depth of focus	11.7 μm	2.1 μm
Beam waist	1.1 μm	1 μm
Laser power	10 mW	9.8 mW
Power density	0.98 MW cm ⁻²	1.1 MW cm ⁻²

FWHM of this curve, one can obtain the DOF of the Gaussian beam. The values for the beam waist and DOF are presented in Table IV. The power used for each objective is also reported in Table IV.

Three Raman spectra were collected from the surface of each sample using the 100× and 50× objectives for strain measurements. The spectrum fitting was performed with a Lorentzian fit to extract the Lorentzian center. The average of these measurements, together with the minimum and maximum values, is shown for the strain evaluation. Both objectives utilized in this study (100× and 50×) have a similar power density on the surface plane of the sample but different power density along the out-of-plane direction. Nonetheless, the power density for both objectives is small, and with the sub-bandgap excitation (532 nm), a negligible self-heating induced by the laser is expected.

For the evaluation of relevant Raman features arising from defects caused by thermal oxidation, the spectral range 1200 to 2000 cm^{-1} was evaluated. The spectra were taken at the surface and at 4 μm depth and were normalized to the highest peak in the range 1200 to 2000 cm^{-1} . Then, the normalized spectra are subtracted from each other. We repeated this process for three distinct regions in each sample and report representative spectra here. This methodology has been previously employed in the literature [27,28]. The normalization of the spectra removes artificial features, and the subtraction allows identification of carbon species, as their spectral position overlaps with the second-order Raman signal of 4H-SiC. The D and G Raman modes for carbon species are located at approximately equal to 1300 and approximately equal to 1500 cm^{-1} [29].

C. DFT calculations

Density functional theory calculations were performed within the Kohn-Sham framework using the Vienna *ab initio* simulation package code [30–32]. Plane waves and the projector augmented wave method [33] were employed to handle valence and core electrons, respectively. Calculations were performed using the R²SCAN meta-GGA functional [34] as it has been found to describe defect energetics and geometry in a satisfactory manner for SiC while keeping computational cost at a reasonable level [35]. Supercells were formed by repeating the 4H-SiC unit cell $6 \times 6 \times 2$ times.

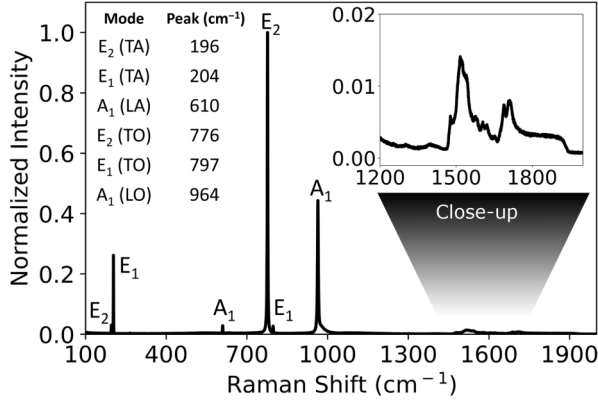


FIG. 2. Raman spectrum for a pristine 4H-SiC sample (Epi_{10 μm}-N₁₅). The inset shows a close-up of the 1200 to 2000 cm⁻¹ region.

Defects were introduced by substituting Si and C atoms by dopant atoms. Al occupies the Si site and N the C site [36], while P can occupy both, but with a preference for the Si site [37,38]. For the defect calculations, the total energy and geometry were optimized using Γ -only k -point sampling, a 1×10^{-6} eV cut-off criterion for the electronic self-consistent loop, a 500 eV energy cut-off and a relaxation criterion for the maximum force of 0.01 eV/Å. Only the ionized charge state, i.e., the charge state after accepting (Al) or donating (N and P) an electron, was considered. The pressure in the supercell calculated before and after introducing the defect is reported.

III. RESULTS AND DISCUSSION

A. 4H-SiC Raman signatures

Typical Raman spectra of 4H-SiC contain first-order and second-order signatures [39,40]. An example is shown in Fig. 2. Since the propagation angle is normal to the sample surface, the observed phonon modes are propagating along the c axis $\langle 0001 \rangle$ [19]. The longitudinal optical (LO) mode A₁(LO), the transversal optical (TO) modes E₁(TO), and E₂(TO) are first-order Raman signatures of 4H-SiC, while the transverse acoustic (TA) modes E₂(TA) and E₁(TA) are the second-order modes of 4H-SiC. The modes present between 1200 and 2000 cm⁻¹, seen in the inset of Fig. 2, are also second-order Raman modes.

The A₁(LO) mode is the LOPC located at 996 cm⁻¹ used previously to calculate the DOF. This mode is sensitive to the free charge carrier concentration [26], as previously mentioned with relation to the DOF measurement. The E₂(TO) mode, located at 776 cm⁻¹, is commonly used to evaluate the strain in 4H-SiC [12,19,41] since it exhibits a frequency shift to lower or higher frequencies in the presence of tensile or compressive strain, respectively [42].

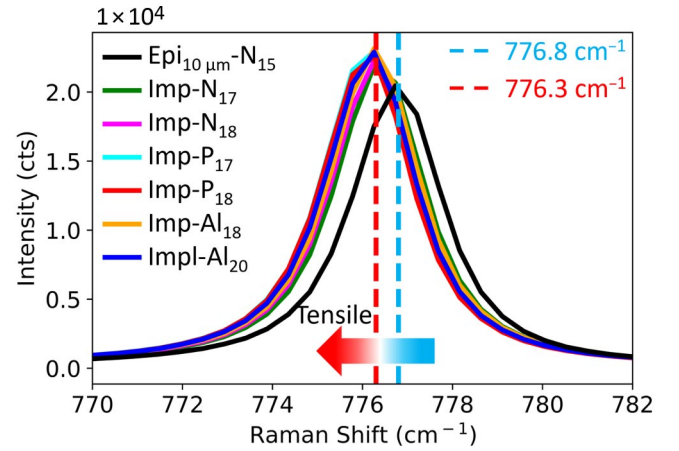


FIG. 3. Raman spectra for pristine (black) and implanted (color) samples in the 770 to 782 cm⁻¹ range using the 50× objective. The spectra for implanted samples exhibit a peak shift which demonstrates the presence of tensile strain in the ion-implanted samples.

B. Strain evaluation

The E₂(TO) mode at 776 cm⁻¹ in 4H-SiC is sensitive to strain in the material. Figure 3 shows Raman spectra for pristine and implanted samples focused on the 776 cm⁻¹ peak obtained using the 50× objective. The spectra for ion-implanted samples exhibit a peak center shift toward lower Raman modes. This shift evidences the presence of tensile strain in the ion-implanted samples as compared with the pristine case. To compare the impact of different processing steps, including ion implantation and thermal oxidation, on strain in the 4H-SiC epitaxial layers, the peak position of the E₂(TO) mode is monitored. Figure 4 shows the variation of the E₂(TO) peak position after ion implantation, thermal oxidation and various heat treatments with respect to the pristine samples (Epi_{10 μm}-N₁₅ for ion implantation and Epi_{30 μm}-N₁₅ for thermal oxidation).

Figure 4 shows the center position of the 776 cm⁻¹ Raman peak for each sample relative to the pristine value, allowing for a comparison of different processing steps, labeled as $\Delta E_2(\text{TO})$. The right-hand y axis reports the estimated corresponding stress (in MPa), obtained by converting $\Delta E_2(\text{TO})$ using the in-plane stress relation reported in Ref. [19], which is based on controlled uniaxial stress measurements along the Z axis. Figure 4(a) highlights the impact of doping by ion implantation of N and P, Fig. 4(b) shows Al-implanted samples, while thermal oxidation related processing steps are summarized in Fig. 4(c). Depending on the processing step either tensile or compressive strain can be observed. The magnitude of the strain is increased for the 50× objective due to the increased probing volume in comparison to the 100× objective, showing that the strain is distributed throughout the epitaxial layer.

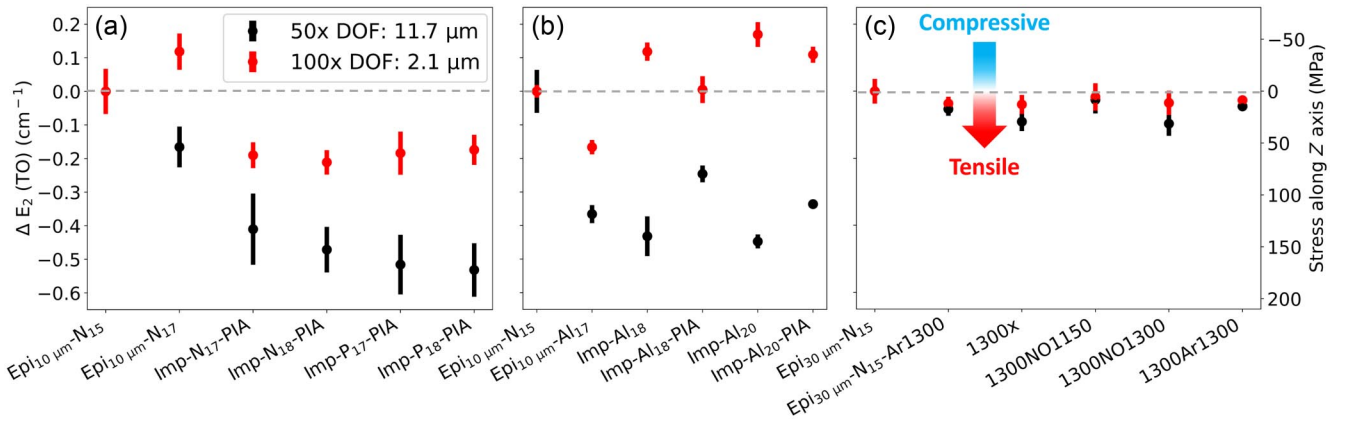


FIG. 4. Shift of the $E_2(\text{TO})$ mode at 776 cm^{-1} , relative to the position measured in the pristine samples. The shift occurs due to the strain induced by ion implantation (a),(b) and thermal oxidation (c). The dashed line indicates the case where no strain is present. The right-hand y axis shows the estimated stress corresponding to the $\Delta E_2(\text{TO})$, calculated using the relation reported in Ref. [19].

Figures 4(a) and 4(b) show a peak shift for highly doped epitaxial layers with $1 \times 10^{17} \text{ cm}^{-3}$ N and Al doping, respectively, as compared with the pristine $1 \times 10^{15} \text{ cm}^{-3}$ doping case (sample $\text{Epi}_{10 \mu\text{m}}\text{-N}_{15}$). This indicates the presence of strain in more highly doped 4H-SiC epitaxial layers, and more precisely tensile strain. It should be noted that sample $\text{Epi}_{10 \mu\text{m}}\text{-N}_{15}$ shows compressive strain for the 100 $\times$ objective, while for the 50 $\times$ objective tensile strain is observed.

For the ion-implanted samples, n-type doping with N and P is depicted in Fig. 4(a) and p-type doping with Al in Fig. 4(b). The influence of the PIA process is illustrated in Fig. 4(b). The N- and P-implanted samples exhibit tensile strain for both probing volumes. Interestingly, the difference between using N and P species is small, but the P-implanted sample has a higher strain compared with the N-implanted samples. Additionally, the higher doping ($1 \times 10^{18} \text{ cm}^{-3}$) exhibits a higher average tensile strain compared with the lower doping ($1 \times 10^{17} \text{ cm}^{-3}$) for both N and P. The Al-implanted samples show tensile strain for the 50 $\times$ objective, at a probing depth of $11.7 \mu\text{m}$, and a compressive strain for the 100 $\times$ objective, at a probing depth of $2.1 \mu\text{m}$. Tensile strain induced by Al implantation has been reported in the literature [43]. The presence of the compressive strain near the surface of the Al-implanted samples can be associated with the formation of an Al complex at the surface, this is elaborated on in Sec. III C. It is observed that after the PIA process, the samples have a lower magnitude of the tensile or compressive strain, showing that the thermal process alleviated the strain in the crystal structure. These results will be put into perspective with DFT calculations in Sec. III D.

For the case of the larger DOF using the 50 $\times$ objective, the magnitude of the strain is larger for the N-ion-implanted samples ($\text{Impl-N}_{17}\text{-PIA}$ and $\text{Impl-N}_{18}\text{-PIA}$) as compared with the pristine N-doped sample ($\text{Epi}_{10 \mu\text{m}}$). This can be associated with the different doping processes.

For epitaxial doping, the N dopants are introduced during the epitaxial growth (without ion implantation). Since no irradiation is performed, the doping during epitaxial growth is likely to produce less strain, which is indeed what we observe for n-type doping, see $\text{Epi}_{10 \mu\text{m}}\text{-N}_{17}$ in comparison to N- and P-implanted samples in Fig. 4(a). However, the highly Al doped epitaxial layer ($\text{Epi}_{10 \mu\text{m}}\text{-Al}_{17}$) follows the same trend as the ion-implanted samples, which can be associated with the larger mass of Al atoms, see Fig. 4(b).

The thermally oxidized samples show tensile strain for both probing volumes, and the results are presented in Fig. 4(c). In comparison to the strain magnitude seen for the ion-implanted samples, the thermally oxidized samples exhibit much lower magnitudes. Previous studies have reported the presence of tensile or compressive strain due to different oxide thicknesses [12]. Herein, we have samples with similar oxide thicknesses (48 up to 56 nm) but different POA processes. The different POA processes induced a small strain and it was not possible to distinguish each thermal oxidation process by Raman spectroscopy.

To investigate the influence of the thermal process (POA or PIA), the sample $\text{Epi}_{30 \mu\text{m}}\text{-N}_{15}\text{-Ar1300}$ was exposed to 1300°C , see Fig. 4(c). The result shows that the temperature alone does not introduce a high tensile strain. Thus, the strains discussed for both ion implantation and thermal oxidation are related to the processing step itself and not the thermal treatment associated with them (PIA or POA).

C. Depth dependent Raman signals

Other than the induced strain by processing steps, Raman spectroscopy can be used to investigate the presence of defect-related vibrational modes within the material as a result of different processing steps. Furthermore, using different objectives allows one to investigate distinct probing volumes within the sample.

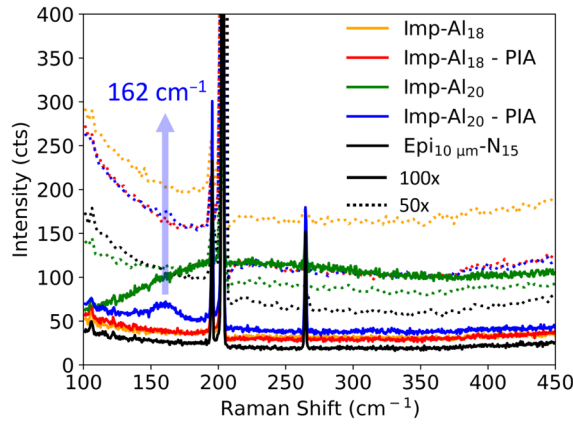


FIG. 5. Raman spectra for the Al-implanted samples with 50 $\times$ and 100 $\times$ objectives showing the appearance of a vibrational mode at 162 cm^{-1} after Al ion implantation to a high density of $1 \times 10^{20} \text{ cm}^{-3}$ followed by PIA (blue curve).

For the Al-implanted samples, a compressive strain was observed for the smaller DOF (2.1 μm for 100 $\times$ objective), while for the larger DOF (11.7 μm for 50 $\times$ objective) only tensile strain was observed. The depth dependent Raman measurements reveal the appearance of a significant vibrational mode at 162 cm^{-1} collected in the near surface region (from the surface up to approximately equal to 2.1 μm) for the high concentration Al ion implantation with PIA (Impl-Al₂₀-PIA), see Fig. 5. The fact that the key vibrational mode is only present after the PIA process can be associated with the energy provided by the PIA to allow the formation of an organized complex. The peak at 162 cm^{-1} is very broad, which indicates that this species is a semicrystalline structure. Previous studies reported on defect formation associated with the Al implantation [23], and structural changes [43,44] induced by Al implantation. In this work, we identified the presence of compressive strain near the surface and a vibrational mode at 162 cm^{-1} induced by the Al implantation. Different from the Al-implanted samples, the N- and P-doped samples do not present structural modifications, thus no relevant depth-dependent Raman signal was identified for the N- and P-doped samples at the doping levels tested here.

As for the thermally oxidized samples, a polyene structure spatially positioned up to 4 μm deeper from the sample surface was identified, see Fig. 6(a) and the subtracted signal in Fig. 6(c). The Raman signature around 1520 cm^{-1} is related to the polyene structure, which is associated with the vibrational mode of a carbon chain [28]. As illustrated in Fig. 6(c), the polyene structure is present independently of the POA process, which indicates a relation to the oxidation process itself and not the subsequent POA process. The other smaller peak at 1750 cm^{-1} shown in Fig. 6(c) can be associated with other amorphous carbon species [29]. The evaluation with the small probing volume, 100 $\times$ objective, depicted in

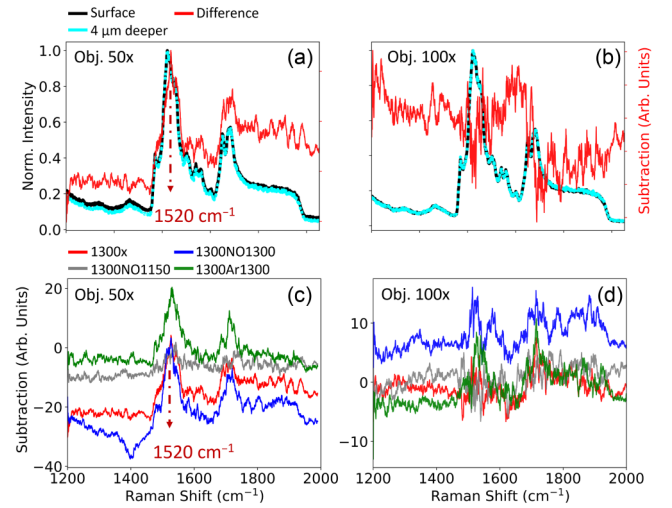


FIG. 6. Evaluation of the depth dependent Raman spectra for the 50 $\times$ objective (a),(c) and for the 100 $\times$ objective (b),(d).

Figs. 6(b) and 6(d) shows that no Raman signature is observed for the conditions used in this work. Since the carbon species are expected to be present within the first few nanometers from the surface and are spectrally positioned at the same location as the second-order Raman modes, their signal gets overshadowed by the signal from SiC [45]. To enhance the surface signal, previous studies have employed the surface enhanced resonant Raman scattering technique to magnify the surface signal [28]. The carbon species detected here is associated with a graphiticlike structure containing polyene and amorphous carbon signatures. No spectral signature from the 2D band of graphene (approximately equal to 2700 cm^{-1}) was observed.

D. DFT calculations

DFT calculations were performed to support the interpretation of strain variations in differently processed SiC as detected by Raman spectroscopy. Table V presents the computed pressure induced by different substitutional dopants on the pseudocubic (k) lattice site in 4H-SiC as compared with the pristine case. In Table V, we consider only the most stable configurations as determined by previous work, i.e., N on C site, Al on Si site, and P on both C and Si sites [36–38]. Only the ionized states ($q = -$ for Al, $q = +$ for N and P) are listed. Since the DFT calculations refer to the ion-implanted regions, we will compare the obtained results with Raman measurements using the 100 $\times$ objective (2.1 μm DOF), which probes mostly the contribution from the ion-implanted regions (100 nm for Al implantation and 300 nm for N and P implantation) and less from the bulk.

Although it does not directly refer to the strain present in the material, the computed pressure values and direction provide an indication of the compressive strain that the

TABLE V. Summary of DFT calculations including pressure computed for pristine supercell versus supercells containing different dopants (Al, N, and P) in their ionized charge states. The pseudocubic lattice site (k) is considered. Positive pressure values refer to compressive strain and negative values to tensile strain.

Defect	Configuration	Charge state	Pressure (kBar)
Pristine	N/A	N/A	1.57
Al _{Si}	k	—	5.97
N _C	k	+	−2.50
P _{Si}	k	+	−2.51
P _C	k	+	2.92

substitutional dopants are imposing on the SiC lattice. Hence, the DFT calculations reveal an increase in the absolute value of supercell pressure as compared with the pristine case for all studied dopants. As can be expected from atom size, the largest effect is found for Al, while N and P have comparable but lower impacts. Interestingly, DFT calculations predict that Al_{Si}(k) imposes a compressive pressure on the lattice, while N_C(k) and P_{Si}(k) cause a tensile pressure. This is in keeping with what is observed for the 100× objective in Figs. 4(a) and 4(b), and supports the interpretation that the opposite Raman shifts observed for Al versus N/P implanted SiC are caused by strain variations. Additionally, the computed positive pressure value for P_C(k) indicates a compressive strain, in contrast to P_{Si}(k), which is associated with tensile strain. This can be related to the slightly lower magnitude of tensile strain observed after P implantation with respect to the N doping [100× objective, see Fig. 4(a)].

IV. CONCLUSIONS

We have investigated the strain induced in the SiC lattice by different processing steps, including ion implantation, thermal oxidation, and thermal processes such as POA and PIA. Raman spectroscopy was able to identify the relative level of strain induced by these processing methods, and the magnitude of the strain was shown to be higher for ion implantation as compared with thermal oxidation. Differences were also found internally within each processing category. Indeed, while N and P ion implantation induce tensile strain in SiC, Al-implanted material exhibits a compressive strain near the surface, which is correlated to the presence of a significant vibrational mode at 162 cm^{−1}. The strain present at the surface of the ion-implanted samples is further confirmed by DFT calculations, which predict compressive and tensile strain in Al and N/P-doped samples, respectively. Furthermore, tensile strain is found to be present after the thermal oxidation steps, however, the strain induced by the different POA processes was too small to distinguish between them. Nonetheless, for all POA processes, a polyene species

located at 1520 cm^{−1} was identified from the surface up to 4 μm deep into the sample. In conclusion, the present work shows that the processing-induced strain in 4H-SiC material can be studied with Raman spectroscopy, a nondestructive technique requiring no previous sample preparation. Beyond quantifying strain variations introduced by implantation, epitaxial growth, oxidation, and subsequent thermal treatments, our results demonstrate that Raman spectroscopy enables the differentiation of strain contributions arising from distinct fabrication steps. Of note, we identify previously unreported Raman modes associated with carbon-related defect species induced by implantation and oxidation, providing insight into structural modifications that extend beyond strain. These findings establish Raman spectroscopy as a powerful diagnostic tool for correlating processing-induced structural changes with material properties relevant to device performance.

ACKNOWLEDGMENTS

The authors acknowledge support from the Scientific Center for Optical and Electron Microscopy (ScopeM) of the ETH Zürich. The work of MEB was supported by an ETH Zürich Postdoctoral Fellowship. Financial support was kindly provided by the Research Council of Norway and the University of Oslo through the frontier research project QuTe (No. 325573, FriPro ToppForsk-program). The computations were performed on resources provided by UNINETT Sigma2—the National Infrastructure for High Performance Computing and Data Storage in Norway. The work of HGM was supported by the Silicon Carbide Qubits toward a Fab-Ready Technology—SiCqurTech (No. SNF 221493).

DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

-
- [1] T. Kimoto, Material science and device physics in SiC technology for high-voltage power devices, *Jpn. J. Appl. Phys.* **54**, 040103 (2015).
 - [2] S. Castelletto and A. Boretti, Silicon carbide color centers for quantum applications, *J. Phys. Photonics* **2**, 022001 (2020).
 - [3] J.-M. Lauenstein, M. C. Casey, R. L. Ladbury, H. S. Kim, A. M. Phan, and A. D. Topper, Space radiation effects on SiC power device reliability, in *Proc. IEEE Int. Rel. Phys. Symp. (IRPS)* (IEEE, Monterey, CA, 2021), pp. 1–8, 10.1109/IRPS46558.2021.9405180.
 - [4] T. Kimoto and H. Watanabe, Defect engineering in SiC technology for high-voltage power devices, *Appl. Phys. Express* **13**, 120101 (2020).

- [5] P. Kumar, M. E. Bathen, M. I. M. Martins, T. Prokscha, and U. Grossner, Electrically active defects induced by thermal oxidation and post-oxidation annealing of n-type 4H-SiC, *J. Appl. Phys.* **135**, 185703 (2024).
- [6] S. Dhar, S. Wang, J. R. Williams, S. T. Pantelides, and L. C. Feldman, Interface passivation for silicon dioxide layers on silicon carbide, *MRS Bull.* **30**, 288 (2005).
- [7] D. M. Fleetwood, 'Border traps' in MOS devices, *IEEE Trans. Nucl. Sci.* **39**, 269 (1992).
- [8] D. K. Schroder, *Semiconductor Material and Device Characterization* (Wiley, Hoboken, NJ, 2015).
- [9] T. Aichinger, G. Rescher, and G. Pobegen, Threshold voltage peculiarities and bias temperature instabilities of SiC MOSFETs, *Microelectron. Rel.* **80**, 68 (2018).
- [10] T. Kimoto, Y. Kanzaki, M. Noborio, H. Kawano, and H. Matsunami, Interface properties of metal-oxide-semiconductor structures on 4H-SiC (0001) and (1120) formed by N₂O oxidation, *Jpn. J. Appl. Phys.* **44**, 1213 (2005).
- [11] P. Kumar, M. I. M. Martins, M. E. Bathen, J. Woerle, T. Prokscha, and U. Grossner, Investigation of the SiO₂-SiC interface using low-energy muon-spin-rotation spectroscopy, *Phys. Rev. Appl.* **19**, 054025 (2023).
- [12] W. Fu, A. Kobayashi, H. Yano, A. Ueda, S. Harada, and T. Sakurai, Investigation of stress at SiO₂/4H-SiC interface induced by thermal oxidation by confocal Raman microscopy, *Jpn. J. Appl. Phys.* **58**, SBBD03 (2019).
- [13] P. Wellmann, N. Ohtani, and R. Rupp, *Wide Bandgap Semiconductors for Power Electronics: Materials, Devices, Applications* (Wiley-VCH, Weinheim, 2021).
- [14] A. Hallén and M. Linnarsson, Ion implantation technology for silicon carbide, *Surf. Coat. Technol.* **306**, 190 (2016).
- [15] R. Nipoti, H. M. Ayedh, and B. G. Svensson, Defects related to electrical doping of 4H-SiC by ion implantation, *Mater. Sci. Semicond. Process.* **78**, 13 (2018).
- [16] J. R. Ferraro, *Introductory Raman Spectroscopy* (Elsevier, Amsterdam, 2003).
- [17] F. Fujie, T. Shiono, K. Murata, N. Ishibashi, Y. Mabuchi, and H. Tsuchida, Formation of basal plane dislocations by stress near epilayer/substrate interface of large-diameter SiC wafers with thick epitaxial layers, *J. Appl. Phys.* **135**, 235701 (2024).
- [18] C. A. Fisher, R. Esteve, S. Doering, M. Roesner, M. de Biasio, M. Kraft, W. Schustereder, and R. Rupp, An electrical and physical study of crystal damage in high-dose Al- and N-implanted 4H-SiC, in *Materials Science Forum* (Trans Tech Publications Ltd., Beach, Switzerland, 2017), Vol. 897, pp. 411–414.
- [19] R. Sugie and T. Uchida, Determination of stress components in 4H-SiC power devices via Raman spectroscopy, *J. Appl. Phys.* **122**, 195702 (2017).
- [20] I. D. Wolf, Micro-Raman spectroscopy to study local mechanical stress in silicon integrated circuits, *Semicond. Sci. Technol.* **11**, 139 (1996).
- [21] G. C. Vásquez, M. E. Bathen, A. Galeckas, C. Bazioti, K. M. Johansen, D. Maestre, A. Cremades, Ø. Prytz, A. M. Moe, A. Y. Kuznetsov *et al.*, Strain modulation of Si vacancy emission from SiC micro- and nanoparticles, *Nano Lett.* **20**, 8689 (2020).
- [22] H. Sakakima, A. Goryu, A. Kano, A. Hatano, K. Hirohata, and S. Izumi, Modeling the effect of mechanical stress on bipolar degradation in 4H-SiC power devices, *J. Appl. Phys.* **128**, 025701 (2020).
- [23] P. Kumar, M. I. M. Martins, M. E. Bathen, T. Prokscha, and U. Grossner, Al-implantation induced damage in 4H-SiC, *Mater. Sci. Semicond. Process.* **174**, 108241 (2024).
- [24] A. Raj, H. A. Witek, and H. O. Hamaguchi, Evaluating stability of a Raman spectrometer for long-time experiments, *J. Raman Spectrosc.* **52**, 1032 (2021).
- [25] S. Fukura, T. Mizukami, S. Otake, and H. Kagi, Factors determining the stability, resolution, and precision of a conventional Raman spectrometer, *Appl. Spectrosc.* **60**, 946 (2006).
- [26] K. Yokomoto, K. Shioura, M. Yabu, M. Nakano, and N. Ohtani, Novel characterization method for the nitrogen doping concentration in heavily nitrogen-doped 4H-SiC crystals by Raman scattering microscopy, *Jpn. J. Appl. Phys.* **59**, 051003 (2020).
- [27] D. Dutta, D. S. De, D. Fan, S. Roy, G. Alfieri, M. Camarda, M. Amsler, J. Lehmann, H. Bartolf, S. Goedecker, and T. A. Jung, Evidence for carbon clusters present near thermal gate oxides affecting the electronic band structure in SiC-MOSFET, *Appl. Phys. Lett.* **115**, 102104 (2019).
- [28] W. Lu, L. C. Feldman, Y. Song, S. Dhar, W. E. Collins, W. C. Mitchel, and J. R. Williams, Graphitic features on SiC surface following oxidation and etching using surface-enhanced Raman spectroscopy, *Appl. Phys. Lett.* **85**, 3495 (2004).
- [29] A. C. Ferrari and J. Robertson, Interpretation of Raman spectra of disordered and amorphous carbon, *Phys. Rev. B* **61**, 14095 (2000).
- [30] G. Kresse and J. Hafner, Ab initio molecular dynamics for liquid metals, *Phys. Rev. B* **47**, 558 (1993).
- [31] G. Kresse and J. Hafner, Ab initio molecular-dynamics simulation of the liquid-metal-amorphous-semiconductor transition in germanium, *Phys. Rev. B* **49**, 14251 (1994).
- [32] G. Kresse and J. Furthmüller, Efficiency of ab initio total energy calculations for metals and semiconductors using a plane-wave basis set, *Comput. Mater. Sci.* **6**, 15 (1996).
- [33] G. Kresse and J. Furthmüller, Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set, *Phys. Rev. B* **54**, 11169 (1996).
- [34] J. W. Furness, A. D. Kaplan, J. Ning, J. P. Perdew, and J. Sun, Accurate and numerically efficient r²SCAN meta-generalized gradient approximation, *J. Phys. Chem. Lett.* **11**, 8208 (2020).
- [35] V. Žalandauskas, R. Silkinis, L. Vines, L. Razinkovas, and M. E. Bathen, Theory of the divacancy in 4H-SiC: Impact of the Jahn–Teller effect on optical properties, *npj Comput. Mater.* **11**, 1 (2025).
- [36] H. H. Woodbury and G. W. Ludwig, Electron spin resonance studies in SiC, *Phys. Rev.* **124**, 1083 (1961).
- [37] S. Greulich-Weber, M. Feege, J.-M. Spaeth, E. N. Kalabukhova, S. N. Lukin, and E. N. Mokhov, On the microscopic structures of shallow donors in 6H-SiC: Studies with EPR and ENDOR, *Solid State Commun.* **93**, 393 (1995).
- [38] A. Fukumoto, First-principles calculations of impurity states in 3C-SiC, *Phys. Status Solidi B* **203**, 125 (1997).
- [39] D. W. Feldman, J. H. Parker Jr, W. J. Choyke, and L. Patrick, Phonon dispersion curves by Raman scattering

- in SiC, polytypes 3C, 4H, 6H, 15R, and 21R, *Phys. Rev.* **173**, 787 (1968).
- [40] S. Nakashima and H. Harima, Raman investigation of SiC polytypes, *Phys. Status Solidi (a)* **162**, 39 (1997).
- [41] M. Yoshikawa, Y. Fujita, and M. Murakami, Stress characterization of the interface between thermal oxide and the 4H-SiC epitaxial layer using near-field optical Raman microscopy, *Appl. Spectrosc.* **73**, 1193 (2019).
- [42] F. Cerdeira, C.J. Buchenauer, F.H. Pollak, and M. Cardona, Stress-induced shifts of first-order Raman frequencies of diamond- and zinc-blende-type semiconductors, *Phys. Rev. B* **5**, 580 (1972).
- [43] K. Piskorski, M. Guziewicz, M. Wzorek, and L. Dobrzański, Investigation of Al- and N-implanted 4H-SiC applying visible and deep-UV Raman scattering spectroscopy, *AIP Adv.* **10**, 055311 (2020).
- [44] J. Muting, V. Bobal, M. G. Willinger, A. B. Zadeh, S. Reidt, L. Vines, and U. Grossner, Spatially resolved diffusion of aluminum in 4H-SiC during postimplantation annealing, *IEEE Trans. Electron Devices* **67**, 4360 (2020).
- [45] J. Woerle, B. C. Johnson, C. Bongiorno, K. Yamasue, G. Ferro, D. Dutta, T. A. Jung, H. Sigg, Y. Cho, U. Grossner *et al.*, Two-dimensional defect mapping of the SiO₂/4H-SiC interface, *Phys. Rev. Mater.* **3**, 084602 (2019).