Study of W centers formation in silicon upon ion implantation and rapid thermal annealing

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Abstract—The recent demonstration of optically active telecom emitters in silicon has paved the way for realizing industrial-scale silicon-based solid-state quantum photonic platforms. The scientific community has been pursuing the implementation of novel single-photon devices for quantum technology applications by introducing extrinsic impurities inside the silicon lattice upon ion implantation. Here we report the optical characterization through single-photon microscopy of intrinsic W centers in highpurity silicon substrates upon carbon implantation and subsequent rapid thermal annealing. The photoluminescence investigation of their emission properties at cryogenic temperatures allowed us to identify the effects of the postimplantation thermal treatment in the formation of telecom quantum emitters based on interstitial silicon clusters upon the introduction of an extrinsic atomic species.

Keywords—quantum photonics, silicon, telecom emitters, rapid thermal annealing, ion implantation

I. INTRODUCTION

Recently it has been demonstrated that silicon can host optical defects with single-photon emission in the near IR [1]. Notably, the W centre is a tri-interstitial complex characterized by a sharp zero phonon line (ZPL) at 1218 nm (1.018 eV) [2]. It is considered to have a trigonal geometry, and five defective alternative configurations of the centre have been proposed so far. Based on classical molecular dynamics (CMD) simulations and density functional theory (DFT) calculations, the so-called I₃-V complex is the most energetically favourable candidate [3]. Furthermore, it has been recently demonstrated that the W center can be isolated at the single-photon emitter level, thus offering an enticing platform for integrated silicon photonics based on native defects. In this perspective, the manufacturing of singlephoton sources based on W centers at the wafer scale relies on the technological capability of their controlled placement in high-purity silicon substrates. For this goal, mature ion implantation techniques are required to deliver single impurities with high spatial resolution. On the other hand, highly efficient post-implantation processes play a crucial role in enabling their optical activation upon conversion into stable lattice defects. So far, W-centre photoluminescence emission optimization has been studied upon silicon implantation to create self-interstitial defects [4]. However, the increasing interest in the scientific

community for realizing novel deterministic silicon-based single photon sources has been pursued by introducing different impurities in the silicon lattice [5]. Therefore, this work investigates the suitability of ion implantation for the fabrication of W centres. The study relies on C keV ion implantation and subsequent multiple-step rapid thermal annealing processes. In this way, these results offer insight into the concurrent kinetics factors involved in incorporating carbon impurities.

II. EXPERIMENTAL

A set of seven 3x3 mm² nominally identical pieces has been cut from a commercially available float zone n-type silicon wafer. 36 keV ¹²C⁻ has been homogenously implanted at 2.10¹⁴ cm⁻² fluence in each of the samples, which have been subsequently thermal processed with a PID-controlled SSI SOLARIS 150 Rapid Thermal Processing System. In this way, we were able to perform seven rapid thermal annealing (RTA) processes at different temperatures: 320°C, 365°C, 400°C, 450°C, 500°C, 700°C, and 1000°C. To investigate the emission properties of the processed substrates, photoluminescence (PL) characterization was carried out at cryogenic temperatures using a custom fiber-coupled single-photon sensitive confocal microscope, where a 488 nm CW laser diode provided laser excitation, and a vacuum-compatible 100× air objective produced a diffraction-limited focused excitation spot on the sample. The latter is mounted on a closed-cycle optical cryostat. A combination of a 700 nm long-pass dichroic mirror and an 800 nm long-pass filter was then used to select the proper spectral range to be investigated. The pinhole of the confocal microscope is represented by a multimode optical fiber which was fiber coupled to an InGaAs single-photon avalanche detector (MPD PDM-IR / MMF50GI). By connecting the confocal microscope fiber output to a Horiba iHR320 monochromator the spectral analysis was finally accomplished with a system spectral resolution evaluated as ≤ 4 nm.

III. OPTICAL CHARACTERIZATION

The photoluminescence (PL) spectra acquired at 10 K following RTA treatment are reported in "Fig. 1" for different annealing temperatures upon an optical excitation power of 4.41 mW. The spectral analysis shows that all of the samples

processed with the 20 s RTA process formed the W centre (corresponding to the sharp emission line at 1218 nm and its phonon replicas at higher wavelengths) for annealing temperatures lower than 450°C. The intensity of the W emission steadily decreases at increasing annealing temperatures, indicating a progressive recovery of the crystal lattice. Regardless of the processing temperature and despite the introduction of carbon impurities employing ion implantation, in contrast to other previously reported investigations on Silicon On Insulators (SOI) substrates [6], no spectral features associated with the carbon-based centres, known as G centres, can be identified at any RTA processing stage. The point defect has been attributed to a neutrally-charged substitutional dicarbon pair coupled to an interstitial silicon atom. This result indicates the G centres' poor formation efficiency under RTA post-implantation treatment in high-purity samples where the low native carbon concentration probably limits its formation. On the other hand, the enhancement of the emission at 1218 nm for lowest considered annealing temperatures demonstrates that the radiation damage introduced upon keV ion implantation is effective at promoting the formation of the W centers and it is consistent with the optimization of photoluminescence from W centres reported upon Si implantation [4].

IV. CONCLUSION

To conclude, we demonstrated that through carbon ion implantation and conventional rapid thermal annealing treatment, it is possible to reliably induce the formation of the W centres in float-zone silicon. The W centre's deactivation and the crystal matrix's complete reconstruction are confirmed for temperatures above 500°C. On the contrary, the lack of observation of any spectral features related to carbon-based optically active defects confirms that in high-purity silicon substrates, the defect evolution pathway (i.e. activation and subsequent deactivation for higher annealing temperatures) is not accessible under stationary thermal treatments at time scales of few seconds.

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Fig. 1: PL spectra of the sample processed with rapid thermal annealing process at different temperatures. All measurements were performed at T=10 K using a 488 nm excitation with an optical power of = 4.41 mW

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