Ion Implantation Point Defect Engineering in SiC for Photonic Quantum Technology

Mathilde BROCHETON^{1,2}, Mihai LAZAR^{1,2*}

¹ Light, Nanomaterials & Nanotechnologies (L2n), CNRS ERL 7004, University of Technology of Troyes, 12 rue Marie Curie, 10004 Troyes, France ² Laboratoire de Recherche en Nanosciences (LRN), Université de Reims Champagne Ardenne, Moulin de la Housse, 51687 Reims, France *E-mail: mihai.lazar@utt.fr (corresponding author)

Silicon carbide, today a largely used semiconductor material in power electronics, has recently shown its potential in photonic quantum technology with its capability to host color centers [1]. Color centers are optically active defects in the lattice of a semiconductor material. Isolated color centers can be used as single photon sources, which have various possible applications for quantum computing technology, quantum cryptography and quantum sensing. The $N_C V_{Si}$ color centers in silicon carbide have properties analogous to well-known nitrogen vacancy (NV) centers in diamond, identified to display single photon emission and long coherence spins, and emit near-infrared light by photoluminescence at room temperature [2]. It consists of a nitrogen substituting a carbon atom (N_C) and a silicon vacancy (V_{Si}) adjacent to it.

In order to obtain the $N_C V_{Si}$ in SiC, its classic n-type dopant is used, the nitrogen, which can be localized in the bulk by ion implantation doping. The nitrogen ion will substitute a carbon of the SiC lattice after thermal post-implantation annealing. The Si vacancy could be generated at the same depth by implantation of another ion with different energy, as carbon (C) ions increasing also the probability to create Si vacancies in the SiC lattice. During the ion implantation process, extremely low doses (10^{12} cm⁻² and even less) are necessary in order to obtain a quasi-individual generation of the defects. Ion implantation will damage the SiC lattice of the crystal along the ion trajectories, a careful thermal annealing is needed to recreate the crystallinity of the material, and to generate the N_CV_{Si} associated defects but without annihilating them.

In order to see how to implement N_CV_{Si} in SiC, we ran ion implantation Monte-Carlo simulations with SRIM [3] and I²SiC[4]. I²SiC exclusively deals with SiC and takes into account its crystalline structure (3C-SiC, 4H-SiC or 6H-SiC) and implantation conditions (polytype chosen, temperature), while SRIM considers SiC as an amorphous material.

For these simulations, the goal was to roughly coincide (with ~75% overlapping) the Si vacancy distribution with previous nitrogen profiles fixed at three different energies: 20 keV, 60 keV and 100 keV. Table 1 presents the optimum energies found for C ion implantations comparing the peak positions and concentrations obtained for an individual dose of 10^{12}cm^{-2} in each case.

Due to the crystal nature of the target (4H-SiC considered here), we can have what is called the channeling effect. It occurs when the direction of the incident ion beam is along one of the crystal basis vector. The implanted ion will interact with quasi-elastic collisions with the atoms of the target, and the energy is mainly dissipated by electronic interactions. In the configuration of channeling effect, the implanted ions will travel a larger distance and less damage through the target. Thus, channeling mode represents a particularly suitable configuration to generate N_CV_{Si} color centers in SiC single-crystal.

When there is a channeling effect, the shape of the implanted ion profiles and generated vacancy concentrations will differ. Two peaks are presents instead of one, the second peak being related to the channeling effect [4]. Figure 1 represents N ions distributions obtained by I²SiC (for 20keV and 60keV) between a disorientated (tilt=8°, rotation=20°) and an aligned configuration corresponding to the channeling effect along the [0001] direction of the 4H-SiC. We note that a quasi-flat profile is obtained at 20keV in channeling mode increasing the window allowed to generate the color centers. Nevertheless, the presence of the two peaks makes calculations more laborious to overlap N and V_{si} profiles (Fig. 2).

Optical properties of these associated defects created by ion implantation in channeling mode and annealed between 800 to 1800°C in a dedicated AET RTP furnace, will be presented at the conference and in the final paper.

Ion	N	C (SiV)
With SRIM		
Energy(keV)	20	24
Max Concentration (cm^{-3})	2.80×10^{17}	2.90×10^{19}
Peak position(Å)	396	371
Energy(keV)	60	65
Max Concentration (cm^{-3})	1.58×10^{17}	2.46×10^{19}
Peak position(Å)	1120	1142
With I ² SiC (8°, 20°)		
Energy(keV)	20	24
Max Concentration (cm^{-3})	2.36×10^{17}	2.00×10^{19}
Peak position(Å)	404	331.4
Energy(keV)	60	65
Max Concentration (cm^{-3})	1.09×10^{17}	1.73×10^{19}
Peak position(Å)	1167	967
With I ² SiC $(0^{\circ}, 0^{\circ})$		
Energy(keV)	20	24
Peak concentrations(cm ⁻³)	8.78×10^{16} and 8.67×10^{16}	4.86×10^{18} and 3.91×10^{18}
Peak positions(Å)	537.6 and 1086	500 and 1300
Energy(keV)	60	65
Peak concentrations(cm ⁻³)	3.00×10^{16} and 6.05×10^{16}	2.94×10^{18} and 3.40×10^{18}
Peak positions(Å)	1306 and 2780	1237 and 2865.6

Table 1: N and V_{Si} peak positions and maximum concentrations; comparing results obtained with SRIM (20 000 implanted ions) and I²SiC with (tilt= 8°;rotation = 20°) configuration and (tilt = 0°; rotation = 0°) configuration in the 4H-SiC polytype, with a dose = 10¹² cm⁻²



Fig1. N profiles obtained with I²SiC for two different implantation energies (20keV, 60keV), on (channeling mode) and off-axis (tilt=8°, rotation=20°) with a dose = 10^{12} cm⁻²; Cat 24 keV (1.10¹² cm⁻³) compared to the N ions distribution at 20 keV [12SiC(0,0)] le16



Fig2. On-axis I²SiC (tilt = 0°, rotation = 0°): Si and C vacancies concentrations created by Carbon ions (dose = 10^{12} cm⁻²) implanted at 24keV, compared to the N profile obtained at 20keV

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