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Correlation between strain and defects in Bi implanted Si

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ABSTRACT

The strain in Si containing group-V impurities is a topical subject of study due to its potential applications in quantum computing. In this paper we study ^{209}Bi implanted Si concerning the correlation between the strain produced by stopped Bi ions and trapping characteristics of the defects resulted from implantation. The depths distributions of stopped ions and primary defects are simulated and the distributions of permanent defects are modelled for Si implanted with low fluence ^{209}Bi ions of 28 MeV kinetic energy. For comparison, these depths distributions were similarly calculated for ^{127}I ions with the same fluence and energy, implanted in Si. The results are compared with each other and correlated with the characteristics of traps in these systems, previously obtained. We demonstrate that the intensity of the strain field is the most important factor in changing of trap parameters, while the superposition between the region with strain and the region where defects are located is a second order effect.

1. Introduction

The system of electron and nuclear spins of donor atoms in silicon is an excellent quantum bit (qubit) candidate for quantum information processing [1,2], and it is expected to be a better solution in respect to superconducting qubits which show relatively fast decoherence rates, insufficient for maintaining quantum information throughout the course of computation. In isotopically enriched ^{28}Si ($I=0$), the coherence times are improved in comparison to natural Si, due to the removal of the residual nuclear spins of ^{29}Si, which has the natural abundance of ~4.7%, and is the only one isotope of natural Si with nonzero nuclear spin ($I=1/2$) [3,4]. The interest in Bi doped Si materials suddenly increased in the last years, based on this potential application. Clock transitions with coherence times of several seconds (at 5 K), much longer than those characterizing superconducting qubits, were reported [5–7]. In parallel, studies on the nuclear spin of ionised ^{31}P donors in isotopically purified ^{28}Si have demonstrated even higher coherence times, in the order of tens of minutes or even higher, at room temperature [8,9]. Recently it was reported that the quadrupolar interaction of group-V donors with nuclear spin $I>1/2$ with electric field gradients can be manipulated by applying elastic strain to the host crystal, for mechanical tuning the nuclear spin of ionised donors [10,11], with the benefit of scalable local addressing the qubits. The strain is applied locally by piezo-actuators on the scale of nanometres in Ref. [10], while in Ref. [11] the defects created during Si implantation modify the nuclear electric quadrupole interaction of the nuclear quadrupole moment with the electron wavefunction. The relation between electric field gradient tensors and lattice strain was theoretically substantiated [12,13] based on experimental data from nuclear acoustic resonance [14]. For Si, this topic only recently appeared in the literature, in relation to the mentioned applications in quantum computing [10].

In the present paper we aim to study the system ^{209}Bi–Si from the point of view of the relation between the strain field produced by Bi ions (bigger and heavier than the Si host atoms) and the trapping properties of the defects produced during Bi implantation, particularly of the relation between strain field intensity and the relative depth distributions of both strain field and defects.

For this, we comparatively analyse Si single crystals implanted with Bi and I ions, both of energy 28 MeV and fluence 5×10^{11} ions/cm^2, which have a lower range than the depth of the samples, and are stopped inside. Both Bi and I ions being bigger and heavier than Si atoms produce a local strain in Si, which is more intense in Bi implanted Si. On the other hand, during their penetration into Si, the ions generate lattice defects. Based on the simulations of depth distributions of stopped ions and of primary defects respectively, we model the production of point defects and their depth distributions. The trap parameters of these irradiation defects were previously obtained by modelling the experimental thermally stimulated current without applied bias curves measured on similar Si samples, implanted with Bi and I ions [15,16], considering the effect of strain. The differences in the characteristics of the trapping centres corresponding to Si samples with Bi and I are correlated and explained based on the results of simulations of ion penetration into Si and on the peculiarities of the fields of strain.

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2. Spatial distribution of the strain fields and defects

The experimental data are from our previous work, Refs. [15,16]. High resistivity Si wafers grown by the floating zone technique, of 2 in. diameter and 280 μm thickness (from Siltronix), contain natural abundances of Si isotopes, *i.e.* 92.2% ^{28}Si ($I=0$), 4.7% ^{29}Si ($I=1/2$) and 3.1% ^{30}Si ($I=0$). They were irradiated with $^{209}Bi^{6+}$ and $^{127}I^{6+}$ ions at the tandem accelerator of Uppsala University [17]. Both ions had the same kinetic energy and fluence of 28 MeV and 5×10^{11} ions/cm^2, respectively. The irradiation nonuniformity on the Si surface was less than 5%, and the beam axis was disoriented in respect to (100) direction by 3° [15,16]. The irradiations were performed at room temperature, and the samples were not annealed for Bi activation [18], but they were kept at room temperature between irradiation and measurements.

2.1. Simulation of Bi^{6+} and I^{6+} ions penetration in Si

The range of both ions of kinetic energy 28 MeV and 3° disoriented in respect to the (100) axis of Si is much smaller than the sample thickness, and consequently they are stopped inside. In order to simulate their penetration into the Si lattice, we used the Monte Carlo code Crystal Transport and Range of Ions in Matter (CTRIM) [19], based on the binary collision approximation. In contrast to the SRIM (Stopping and Range of Ions in Matter) code [20] that simulates the penetration of ions in amorphous targets, CTRIM takes into account the crystal structure and the orientation of the ion beam in respect to the lattice. So, the programme follows the incoming particle and all the particles it sets in motion until they fall below a selected low kinetic energy. It is known that the competition between nuclear and electronic stopping for different ions is a function of ion characteristics (charge and mass numbers) and energy. So, when entering the sample, both Bi and I ions lose energy predominantly by ionisation. Being lighter, I ions penetrate farther into Si. It is known that with the increase of the atomic mass and charge numbers of the ion, the maximum of the nuclear energy loss is shifted to higher energies, and the value of the maximum is also higher, this being correlated with a higher displacement damage production. The nuclear energy loss is the highest near the end of the range, *i.e.* at low ion energies, and consequently in this region the concentration of defects is also higher, as it will be seen further.

In the following, we are interested only in distributions in the depth of the sample, due to the uniformity of the irradiation on the surface. The distributions of stopped ions are nearly Gaussian, with the maxima located at 4.77 and 8.36 μm for Bi and I ions, respectively [15,16]. These distributions are illustrated in Fig. 1, where the centre (projected range) and the standard deviations (range straggling) of each of them are marked. One can see that the distribution of Bi ions is much narrower, steeper than the distribution of I ions.

Each stopped ion, being bigger ($r_{Bi}=1.70$ Å and $r_I=1.28$ Å) and heavier ($A_{Bi}=209$ and $A_I=127$) than the atoms of the host lattice ($r_{Si}=1.17$ Å, $A_{Si}=28$) produces a local deformation of the lattice. The strain fields produced by all stopped ions add together. The two ions, Bi and I, being differently distributed in the depth of Si, create different configurations of the field of strain. So, the departure of each of the ions studied from the Si atoms of the host lattice (mass, size, electronic configuration) is different, and it is expected that the magnitudes of created strain are also different.

2.2. Simulation of the distributions of primary defects produced by Bi and I ions in Si

The depth distributions of the vacancies created by the two types of ions, as a consequence of the energy transmitted to the atomic motion, as obtained from CTRIM are represented comparatively in Fig. 2. These distributions are asymmetrical, with the maxima situated at 4.25 μm and 7.35 μm, giving a total number of vacancies

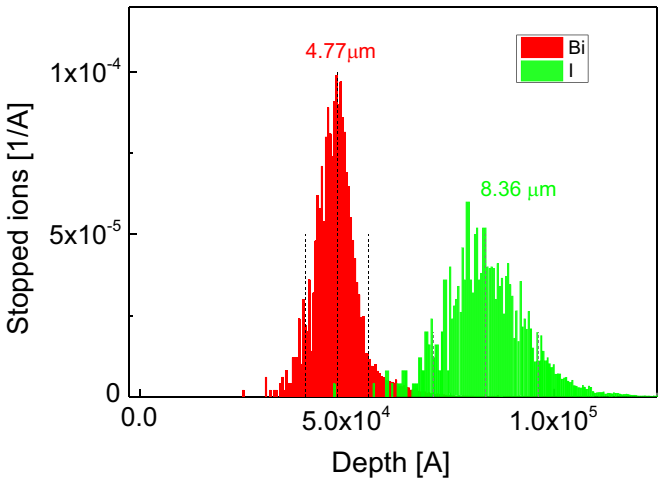

Fig. 1. Depth distribution of stopped Bi and I ions, with the projected range and standard deviation (range straggling) marked.

per ion of 7.17×10^4 and 5.72×10^4 for Bi and I ions, respectively. The asymmetry of the distributions of vacancies, i.e. their tails toward the sample surface, is explained by primary defects (vacancies and interstitials) creation in atomic collision cascades, having the source in the primary knock-on atoms. So, in each interaction, if the energy transmitted to the atom exceeds the threshold energy for displacements, the atom leaves its site in the lattice, creating a vacancy–interstitial pair. The self-interstitial, which is the recoil created in the primary interaction, can be the source of a cascade of displacements if it has enough energy. Hence near the trajectory of the heavy ion, vacancies and interstitials are created in pairs.

2.3. Modelling of the distributions of stable defects following Bi and I irradiation

As in Si both interstitials and vacancies have a very fast and long range migration [21], they interact either between themselves or with the defects and impurities present in the lattice via migration, recombination and annihilation, thus forming stable point defects which are related to interstitials or to vacancies. The main impurities present in our samples are O, C (both with concentrations in the order of 10^{15}–10^{16} at/cm^3) and P (5×10^{11}–5×10^{12} at/cm^3). In the frame of the theory of diffusion – limited reactions, the process of

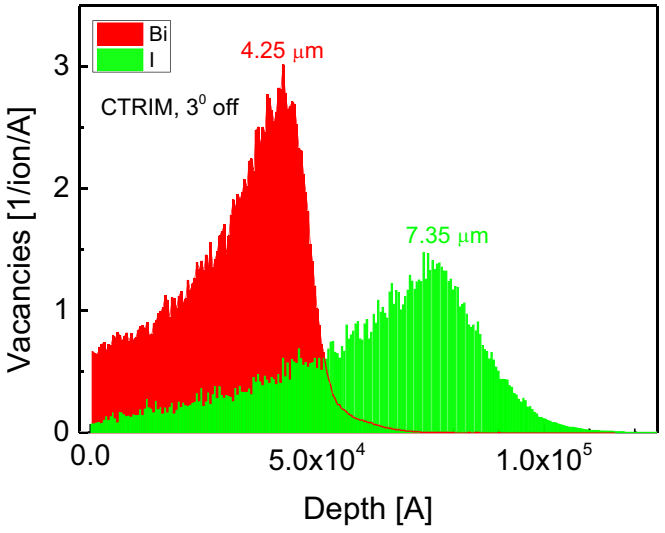

Fig. 2. Depth distribution of vacancies created in Si following the irradiation with Bi and I ions, of 28 MeV kinetic energy.