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Investigation of amorphization energies for heavy ion implants into silicon carbide at depths far beyond the projected ranges

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ABSTRACT

At ion energies with inelastic stopping powers less than a few keV/nm, radiation damage is thought to be due to atomic displacements by elastic collisions only. However, it is well known that inelastic processes and non-linear effects due to defect interaction within collision cascades can significantly increase or decrease damage efficiencies. The importance of these processes changes significantly along the ion trajectory and becomes negligible at some distance beyond the projected range, where damage is mainly caused by slowly moving secondary recoils. Hence, in this region amorphization energies should become independent of the ion type and only reflect the properties of the target lattice. To investigate this, damage profiles were obtained from α-particle channeling spectra of 6H-SiC wafers implanted at room temperature with ions in the mass range $84 \leqslant M \leqslant 133$, employing the computer code DICADA. An average amorphization dose of (0.7 ± 0.2) dpa and critical damage energy of (17 ± 6) eV/atom are obtained from TRIM simulations at the experimentally observed boundary positions of the amorphous zones.

1. Introduction

Silicon carbide is an important ceramic material with many technological applications ranging from cladding material of nuclear fuel elements to electronic devices in high-temperature and harsh radiation environments. Its thermal stability and especially its amorphization properties during ion implantation have therefore extensively been investigated. Although irradiation-induced amorphization at typical ion implantation energies is primarily caused by displacements during ballistic collisions, results also point to an influence of inelastic processes on damage creation [1,2]. A direct determination of their importance was obtained from an analysis of critical damage energies involved in the production of buried graphitized layers in diamond by C^+ ions [3–5]. It revealed a significant defect annealing effect by electronic stopping, leading to strongly reduced damage efficiencies. However, a similar investigation of damage creation in silicon carbide showed the opposite effect. In this case damage efficiency is strongly enhanced by electronic stopping, leading to lower amorphization energies [6], which might be explained by a reduction of binding energies due to electronic excitation or ionization of target atoms. A comparative study showed that in mono-elemental targets the annealing effect generally dominates, while in binary targets both opposing effects are important, leading either to an enhanced or reduced damage efficiency depending on implantation parameters [7]. In silicon carbide, enhanced damage efficiency is generally observed with increasing electronic stopping [6,8]. However, the importance of the inelastic processes reduces significantly along the ion trajectory, as it depends not only on the ion's mass but also on its velocity. Furthermore, at some distance beyond the projected range ion properties become unimportant, as ions and primary knock-on atoms do not reach this depth and damage is only caused by slowly moving secondary recoils.

Fig. 1 illustrates this situation for the case of strontium ions implanted at 360 keV, using version 98.01 of the well-known pseudo Monte Carlo simulation TRIM [9]. This code employs a universal atomic potential and makes use of statistical distributions of free path lengths and collision parameters for amorphous matter, which makes it much faster than a proper Monte Carlo simulation. High computing speed was essential for this investigation, as about 10^5 ion trajectories had to be simulated using the full-cascade option to obtain the desired statistical certainty at the appropriate depths. The inelastic energy transfers due to the ion and recoiling atoms are shown together with the simulated and experimental implantation profiles in relative units.

Up to a depth of the projected range at 130 nm the total inelastic energy density is relatively high and can significantly influence damage production by the two competing processes of binding energy reduction and defect annealing. The first process, due to the electronic excitation of lattice atoms, causes an increased

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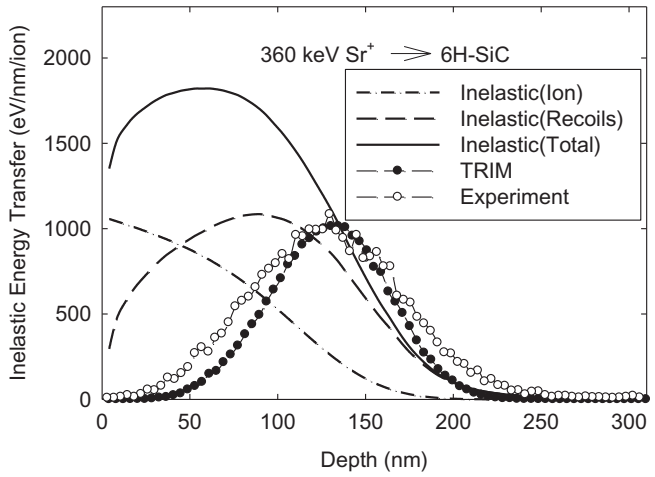

Fig. 1. TRIM-simulation of inelastic energy transfers for 360 keV Sr^+ ions in 6H-SiC together with the calculated and experimentally obtained implantation profiles in relative units.

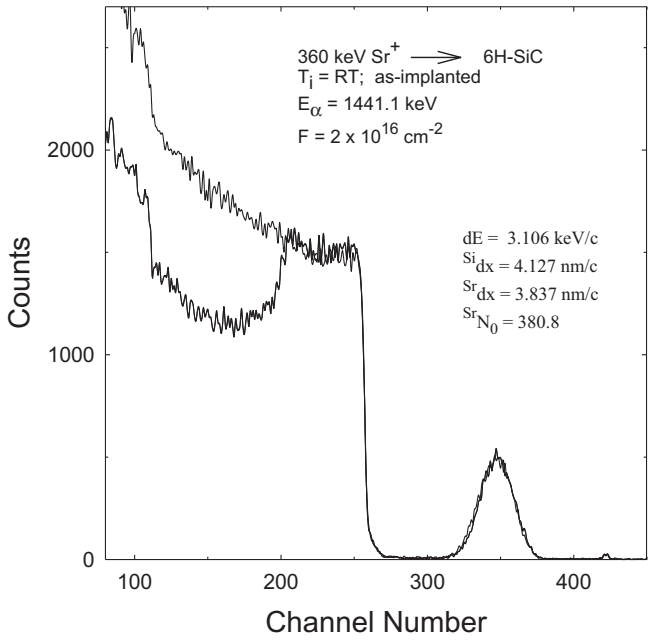

Fig. 2. Random and aligned backscattering spectra of 6H-SiC implanted with 360 keV Sr^+ at room temperature with a fluence of 2×10^{16}.cm^{-2}. The first three numbers in the inset are the energy resolution and the depth resolutions for silicon and strontium per channel, while the fourth is the channel number of the strontium surface.

atomic displacement rate and therefore a lower amorphization dose, while the opposite process of damage annealing will increase the amorphization dose. Damage annealing at inelastic energy densities encountered in this investigation is probably only due to irradiation-induced defect mobility. The effect of heat spikes, which can significantly increase damage recovery, is only expected at inelastic energy densities above approximately 5 keV/nm [10].

At a depth of approximately twice the projected range the contributions from the ion is zero and even those of the recoils becomes small. Contrary to the surface region, where heterogeneous amorphization is observed due to the occurrence of high-defect density islands produced in collision cascades [11], progressive defect accumulation by low-energy elastic collisions, not influenced by inelastic processes or non-linear effects, is expected in this region. This should cause homogeneous amorphization after a critical defect density is reached.

2. Experiment and analysis

To obtain amorphization up to depths of approximately twice the projected range, fluences of the order of 10^{16} cm^{-2} of Kr, Sr, Ag, I, Xe and Cs ions are implanted at room temperature with an energy of 360 keV in hexagonal 6H-SiC wafers from *Intrinsic Semiconductors*®. Typical random and aligned backscattering spectra along the (0001) direction are presented in Fig. 2 for the strontium implant, showing an amorphous region extending from the surface to a depth of 227 nm at a projected range of 130 nm. The integrated yield of the implanted ion species agreed within experimental uncertainty in all cases with the nominal fluence, which is used in all calculations. More details of the experimental method used are reported elsewhere [12]. Damage profiles where obtained from the channeling spectra using the computer code DICADA [13], which makes use of a modified master equation approach based on the channeling concept of the Lindhard theory. The latter theory under-estimates the yield of the aligned spectrum because of the assumption that conservation of transverse energy in an ideal crystal holds right from the surface, while this is only true after the ions have penetrated a relatively large number of atomic layers. This is rectified in the modified master equation by using start values for the minimum yield at the surface obtained from a full Monte Carlo simulation. DICADA calculations can be applied to compounds containing different kinds of point defect configurations, including clusters and amorphous zones, but do not take into account stacking faults and dislocation loops, which have relatively large de-channeling cross sections, leading to artificial tail-effects at larger depths. Assuming randomly displaced atoms, this effect was observed in all samples. To include extended defects, a modified version is used, which originally had been developed for mono-elemental targets only [14,15]. For the current calculations a Debye temperature of $\theta_D = 1030$ K is used, which is an average of the widely varying published values [16]. Furthermore lattice parameters of $a = 0.3081$ nm, $c = 1.5092$ nm and an atomic density of $\rho = 9.662 \times 10^{22}$ at cm^{-3} were assumed. Relative damage densities of the total damage, not corrected for de-channeling effects of

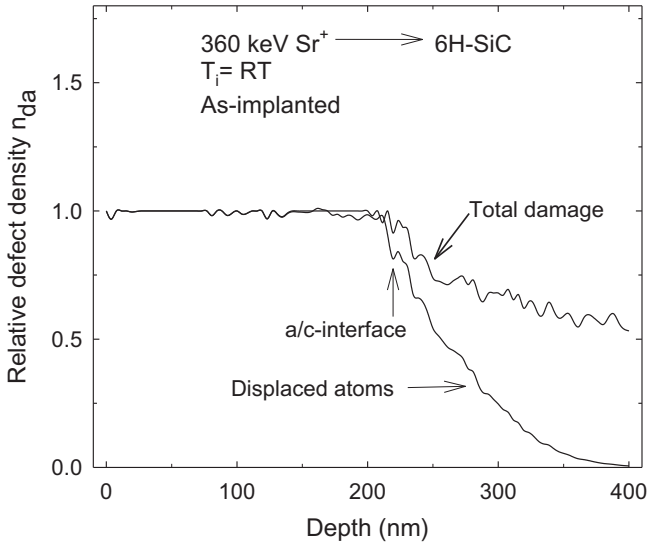

Fig. 3. Relative defect density distributions for the total damage (not corrected for de-channeling effects of extended defects) and for randomly displaced atoms, obtained from the spectra of Fig. 2 using the DICADA code.