Molecular Dynamics Modeling of Octadecaborane Implantation into Si

Luis A. Marqués, L. Pelaz, I. Santos, P. López, and M. Aboy

Department of Electronics, University of Valladolid, 47011 Valladolid, SPAIN
lmarques@ele.uva.es

Abstract

We have carried out molecular dynamics simulations of monatomic B and octadecaborane cluster implantations into Si in order to make a comparative study and determine the advantages and drawbacks of each approach when used to fabricate shallow junctions. We have obtained and analyzed the doping profiles and the amount and morphology of the damage produced within the target. Our simulation results indicate that the use of octadecaborane clusters for the implantation process shows several advantages with respect to monatomic B beams, mainly related to the reduction of channeling and the lower amount of residual damage at the end of range.

1 Introduction

Boron ion implantation has traditionally been used for the fabrication of shallow junctions in MOSFET devices. As technology scales down the energies necessary to fabricate these junctions, monatomic B implantation shows several shortcomings, mainly related to production-throughput and ion-beam high-energy contamination [1]. Implantation of B clusters has been proposed as an alternative to overcome these drawbacks [2]. Recently, the fabrication of nanometric MOSFET devices has been successfully demonstrated [1,3] by using implantation of octadecaborane, a molecule with 18 B atoms [4].

When fabricating a shallow junction it is important to control not only the dopant profile, but also the amount and type of damage generated during the implantation process. A subsequent anneal is carried out to allow the dopants to diffuse to substitutional sites and so become active, and for the lattice defects to recombine. But this process is highly transient and it is governed by the diffusion and complex interactions between dopants and defects, and especially by their clustering. In particular, interstitial defects produce the so-called transient enhanced diffusion (TED) of B, which alters the junction depth [5]. The amount of TED depends mainly on the net excess of interstitial defects at the end of range (EOR) and their proximity to the target surface [6].

We have carried out molecular dynamics (MD) simulations of monatomic B and octadecaborane cluster implantations into Si in order to make a comparative study and so determine the advantages and drawbacks of each approach. Apart from the doping profiles, we will pay special attention to the origin, type, amount and morphology of the damage produced within the target.

2 Simulation Details

We have used the Tersoff multi-component potential [7,8] to describe the Si-Si, B-B and Si-B interactions. We have used Si targets consisting of 32,000 atoms for monatomic B implantations and 600,000 for B_{18} cluster implantations. Ions are implanted with normal incidence on the (100) Si free surface, while periodic boundary conditions are applied in lateral directions. In order to make a statistical study we have carried out 1000 simulations of monatomic B implantations and an equivalent of 56 of B_{18} cluster implantations. Ion impact points are randomly chosen along the target surface, and in the case of B_{18} we initially set the B atoms in agreement with the octadecaborane molecule geometry [4], with random rotations around the three molecular axes. Every B atom has an initial energy of 500 eV, a typical value used nowadays for the fabrication of shallow junctions [3]. Damage resulting from the simulations is characterized by searching target atoms displaced from perfect lattice positions.

3 Results and Discussion

Figure 1 shows two snapshots of final system configurations obtained after typical monatomic B and B_{18} cluster implantations. In the monatomic case damage consists of point defects and small disordered zones, which are the result of the development of the collision cascade initiated by the ion [8,9]. Its interaction with target atoms often generates recoils which leave a vacancy behind and generate an interstitial defect where they stop after losing their energy. On average, each 500 eV monatomic B implant produces 32 displaced atoms. In turn, for B_{18} a big amorphous zone is generated. Almost 70% of the implanted B atoms end within this disordered region. A closer look reveals that this amorphous zone is in fact a crater with the typical rim on the surface. On average, the number of displaced atoms per implanted B is 108, more than three times the number obtained in monatomic B implantations. In this case the origin of damage is related to the simultaneous deposition of energy carried by the B_{18} cluster on the surface region, which causes a crystal-to-liquid transition and, upon cooling, the formation of big amorphous pockets in the cascade core [10].

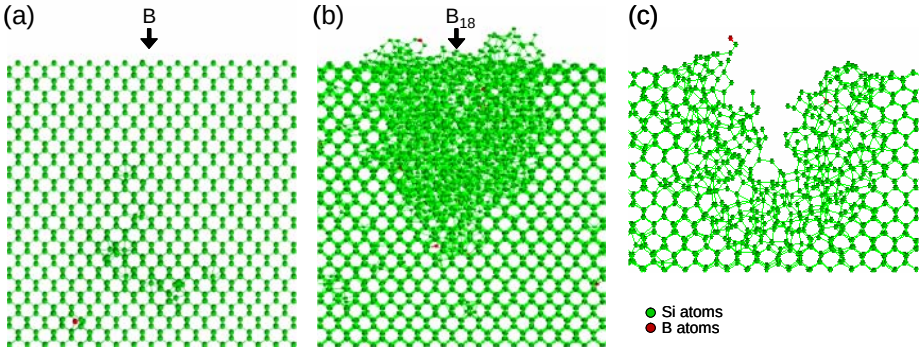

Figure 1: Lateral snapshots with the typical damage configurations obtained after implantations of (a) monatomic B, and (b) a B_{18} cluster. (c) is a thin slice taken from (b) to show the generated crater.

Dopant and damage profiles obtained from the MD simulations of monatomic B and B_{18} cluster implantations are shown in Figure 2(a). Boron profiles are very similar except for a larger tail in the monoatomic case due to channelling. Self-amorphization during cluster implantation causes that less B atoms reach the EOR zone. Damage profiles are in turn very different. Figure 2(b) shows how damage is distributed in interstitial and vacancy defects as a function of depth. Monatomic B mostly produces single and di-interstitials, and small vacancy clusters in crystalline Si. The amount of Si interstitials is larger than that of vacancies, except at the surface. In turn, the dominant defect for B_{18} implants is a large vacancy-rich amorphous pocket (the crater) which is concentrated within 4 nm to the surface. In turn, there is less damage at EOR where channeled B lies.

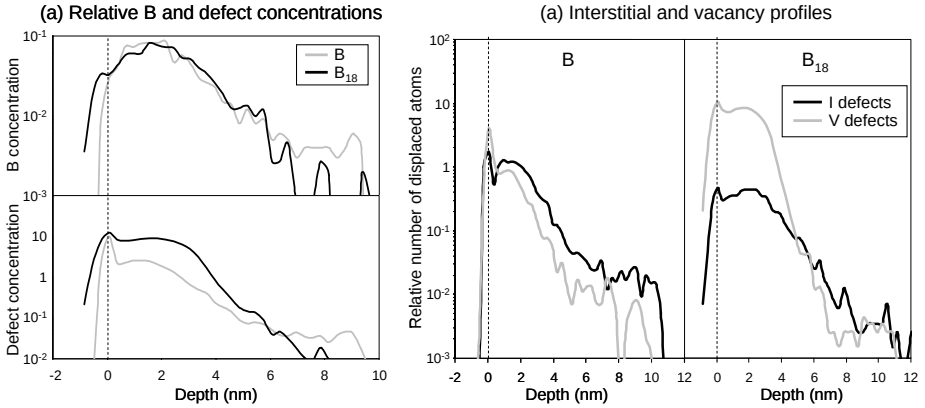

Figure 2: Dopant and damage (a) and defect type (b) profiles obtained for monatomic B and B_{18} cluster implantations.

Upon annealing, excess Si interstitials in the monatomic case will cause TED and clustering, and consequently the spreading and deactivation of dopants. In the B_{18} case, most damage is concentrated at the amorphous pocket. Figure 3 shows three snapshots taken during the annealing of damage produced by one of the B_{18} implants. The underlying crystal substrate serves as a seed for the recrystallization process. At the end, the amorphous region has recrystallized completely. Only point defects outside the initial amorphous zone remain. It is worth to note that B atoms inside the amorphous zone are not swept by the amorphous/crystal interface, and eventually they all end up in substitutional positions.

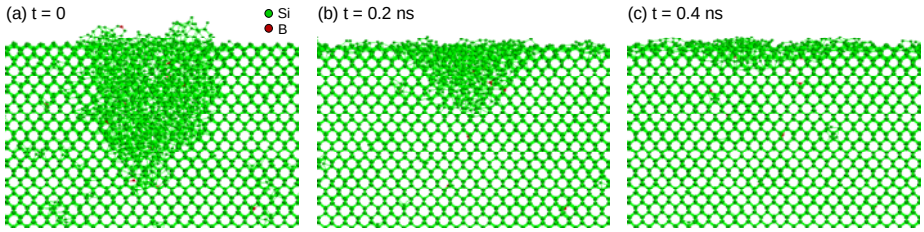

Figure 3: Lateral snapshots taken during annealing of B_{18} implant induced damage.

4 Conclusions

We have carried out MD simulations of monatomic B and B_{18} cluster implantations into Si in order to make a comparative study. From our simulations we have analyzed the mechanisms of defect formation, the profiles of implanted B and generated damage and the morphology of these defects. We have demonstrated that the use of B_{18} clusters to fabricate shallow junctions shows several advantages compared to monatomic B beams. One is the self-amorphization of the target which reduces channeling, so that it is not necessary a pre-amorphization step. The formed amorphous layer is very shallow (4 nm thick), so it can be annealed out with a short thermal treatment. The remaining EOR defects are very close to the target surface, which requires lower thermal budgets to their elimination. Besides, the net amount of interstitial defects in this region is lower, and so will be the TED of dopants.

Acknowledgements

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