Ion Implant Simulations: A kinetic Monte Carlo annealing assessment of the dominant features

I. Martin-Bragado,* M. Jaraiz, P. Castrillo, R. Pinacho, J.E. Rubio, and J. Barbolla
Dept. de E. y Electrónica, Univ. de Valladolid. ETSIT Campus M. Delibes, 47011 Valladolid, Spain
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The atomistic, physically-based kinetic Monte Carlo method has been used in conjunction with the binary collision approximation (BCA) to elucidate the implant mechanisms most relevant for modeling transient enhanced diffusion (TED). For the cases studied we find that: (i) the spatial correlation of the interstitial, vacancy (I,V) Frenkel pairs is not critical, (ii) the interstitial supersaturation in simulations which include full I,V profiles or only the net $I-V$ is the same, (iii) quick and noisy BCA implant I,V distributions can be directly used (or after smoothing them out) as they can still yield accurate annealing simulations, and (iv) when there is an impurity concentration comparable to the net $I-V$ excess, the full I and V profiles have to be used in order to correctly reproduce the impurity clustering/deactivation. Finally, some practical implications for TED simulations are drawn.

Ion implantation is the standard process to establish dopant profiles, which in turn determine the electrical characteristics of devices in integrated circuits. However, the implant process creates extra interstitial (I) and vacancy (V) defects inside the crystal, some of them through replacement of the implanted ions, others from Frenkel I,V pairs (FP). Post-implant anneal processing cures this damage, but the presence of these extra Is cause transient enhanced diffusion (TED), which is a major drawback in the processing of I-mediated diffusing species[1].

To correctly account for TED, process simulators usually generate the damage distribution either by means of an analytical approximation or with a binary collision approximation (BCA) code. This damage has two components, one is the Frenkel pair I and V distributions, the other is an I distribution in a one to one correspondence with the implanted ions (for substitutional impurities). The "+1" model[2], proposed in the early 90's, assumes that the Frenkel pair Is and Vs recombine locally in the bulk and therefore only the extra Is (the ion component) will induce TED until they are finally annihilated at the Si surface. Despite its simplicity it was very successful for boron, for example, under certain conditions but in general it needs to be modified to a "+n" model for other ions or conditions[3, 4].

In this work we have used atomistic non-lattice kinetic Monte Carlo (kMC) simulations to carry out a thorough analysis of this issue. The kMC physically-based method provides exceptionally detailed and realistic simulations that help understand the underlying mechanisms and, thus, allow for simpler but accurate models to be derived. Is and Vs are given random jumps at a rate derived from their diffusivities. The model includes interactions between the particles leading to clustering and re-emission from clusters, trapping and detrapping with impurities. The rates of these processes are determined by specific binding energies derived from molecular dynamics, first principles calculations and experiments[5]. Unlike lattice kMC (see for instance Ref. 6) non-lattice kMC accounts for all possible microscopic configurations of a given cluster size through a single, effective binding energy. This has proven to be enough for the simulation size and time scales involved in typical processing conditions with[7] and without[8] impurities. In particular the activation energy for I emission from a I cluster of size n is calculated as the simple sum of the binding energy plus the I migration energy. The I migration and binding energies (E_b) used are the same as in Ref. 9, which yield good {311} dissolution results, and V binding energies are taken from Ref. 10. The emission prefactor is proportional to the cluster surface, in correspondence with the capture process. Nevertheless, the E_b values would affect the time scale, but not the number of diffusion hops that the particles perform until they are finally annihilated at the surface or recombine with one another. In fact, as we will discuss below, even if the V clusters are not formed at all ($E_b = 0$) the I time evolution is the same.

The initial coordinates of the particles are provided by a BCA simulator. Alternatively, they can be generated at random following the concentration distribution of an input profile. The first topic that we address is the relevance of the spatial correlation of FPs: is the initial distance between each I and its corresponding V relevant or can we get the same TED annealing results by using as input the Is and Vs randomly generated from the concentration profiles? After that, we evaluate the relative weight of the two components of damage, FP and ion. We also show that, for TED simulations, even rather noisy damage profiles, generated with a quick, small BCA implant simulation, can be used to get accurate TED results. Finally, the presence of a substantial amount of impurities is also considered.

As a typical medium energy, medium dose, room temperature implant, we simulate 40 keV, $5 \times 10^{13} cm^{-2}$ Si self implant and a subsequent anneal of 6000 seconds at 738° C. The simulation box surface is $50 \text{x} 50 \text{nm}^2$, which

*Electronic address: ignacio.martin@tel.uva.es

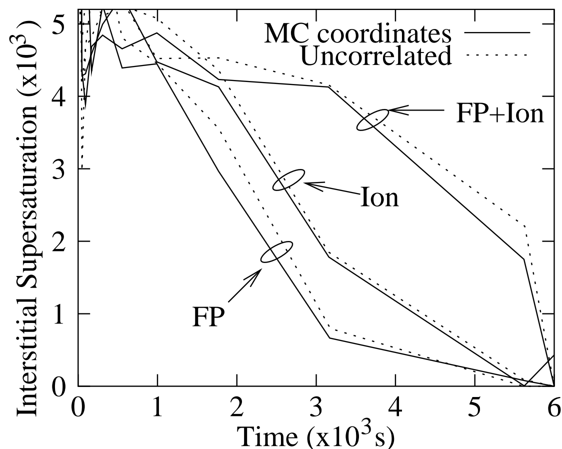

FIG. 1: Interstitial supersaturation time evolution during the annealing at 738° C of a 40 keV, 5×10^{13} cm^{-2} Si implant. The ion component corresponds to the implanted ion ('+1" model) and FP to the damage (FPs) generated by the ion. Solid lines: obtained by reading BCA implant coordinates. Dashed lines: obtained by reading the implant profiles and generating random coordinates.

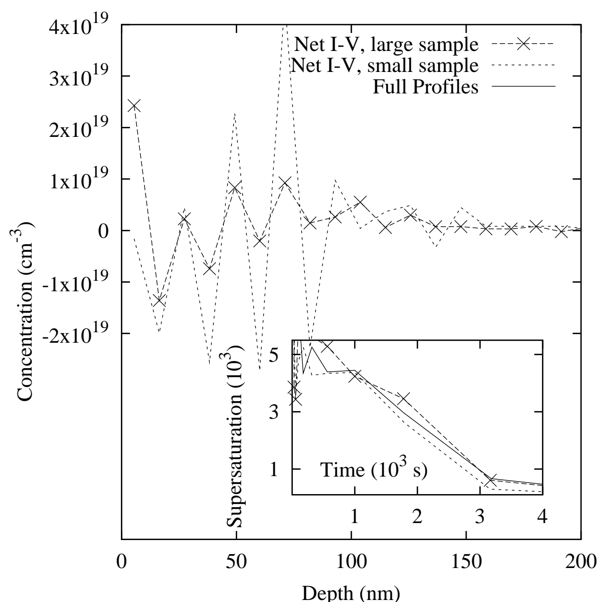

FIG. 2: Dashed line: Very noisy $I-V$ profile from a small ($\approx$ 110 cascades) BCA implant simulation of Si, 40 keV, 5×10^{13} cm^2. Symbols: Same profile for 14500 cascades. Inset: The supersaturation for the small $I-V$ sample (dashed line), for the large one (symbols) and for the full I, V profiles (solid line) is practically the same.

implies the implantation of approximately 1250 ions. The cascades are simulated with the BCA implant simulator MARLOWE[11] and the coordinates of Is and Vs are transferred to the atomistic kinetic Monte Carlo code DADOS[5] to simulate the anneal.

To test if the FP spatial correlation is relevant we compare the annealing results of simulations done using the BCA generated particle coordinates with simulations done using as input the I,V profiles built with those coordinates. Since the code that translates the concentration profiles into discrete atoms in DADOS generates the particle coordinates using a random number generator, all the FP spatial correlation is lost. Also, to see the different contributions to the I supersaturation (the ratio between the concentration of I and its equilibrium concentration), we compare simulations performed with the ions only with simulations carried out with the FPs only. Figure 1 shows the time evolution of the I supersaturation. The I excess decreases when Is recombine with Vs or are annihilated at the surface. The IV recombination events are mostly local and therefore fast. In consequence the excess Is that go up to the surface are the main contribution to the supersaturation.

The time integrated supersaturation for the ion only and for the FPs only, add up to roughly the FP+ion simulation case. However, as it can be seen from the figure, the time evolution is delayed for the FP+ion case. This is due to the ripening of clusters to large, more stable sizes. From Fig. 1 we can conclude that for the conditions studied: (i) The IV spatial correlation is not relevant; it is lost by reading the profiles and yet similar supersaturations are obtained. This fact validates the use of I,V profiles, which is much faster (using analytic approximations) than generating the cascades with a BCA program. (ii) The supersaturation due to the ion is dominant over the one due to FPs, corroborating the "+1" model.

To further test the idea that most Is and Vs recombine locally we have carried out another simulation in which the Is and Vs are only the net local I or V excess. The supersaturation produced is the same, indicating that the number of jumps that the Is perform to recombine locally with Vs is negligible. In addition the number of net Is and Vs is very small compared with their total number, allowing for a less demanding kMC simulation.

When we perform the annealing of a noisy $I-V$ profile i.e., using a very few cascades BCA implant simulation (Fig. 2), the supersaturation obtained is very similar to the one produced by a much larger BCA implant simulation, indicating that the net $I-V$ needed to get the correct supersaturation can be estimated from a quick, although noisy, BCA simulation. The randomization of the diffusion process smears out any BCA noise fluctuation, and the noisy $I-V$ still conveys enough information on the dominant mechanisms that control TED.

When modeling damage anneal in the continuum approach, it is advantageous not to include V clusters to reduce the number of equations, because usually these V clusters do not alter the I supersaturation significantly. Performing simulations with and without the V cluster model, we have verified that the time evolution of the supersaturation is essentially the same. For middle and low implant energies the V clusters are close to the surface, and then the number of jumps that an I performs to be annihilated at the surface or at a V cluster are similar.

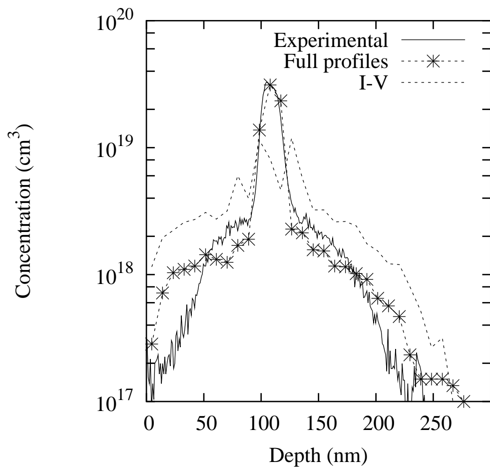

FIG. 3: Simulated and experimental profiles of a $4.5 \times 10^{19}\,cm^{-3}$ B spike after 40keV, $9 \times 10^{13} cm^{-2}$ Si implant and 50 s anneal at 800 ^{o}C. Solid line: experimental data[7]. Dashed lines: Simulations with full I,V profiles and with only the net $I - V$ profiles. Notice that the net $I - V$ profiles do not correctly immobilize the B spike.

For very low doses, for which there is no cascade overlap, other issues besides the FP correlation may come into play. Namely, the individual cascade localization is not reproduced by uniformly randomized concentration profiles[12].

Finally, the presence of impurities can affect the anneal results. As an example we consider boron, which is known to react with Is creating BI clusters (BIC) which play a key role in B diffusion[7]. We have carried out some simulations to help clarify how the previous conclusions can be affected by the presence of impurities. The interaction between a B atom and a Si self-interstitial is described in terms of kick-out and clustering mechanisms[7], with numerical values that yield diffusivity in agreement with Ref. 13.

Fig. 3 shows a B spike, initially from 100 to 120 nm and 4.5×10^{19} cm^{-3} concentration, annealed for 50 s at 800° C after a 40 keV, $9 \times 10^{13} cm^{-2}$ Si implant. We have done the following simulations: (a) using the full I, V implant profiles, and (b) using only the net I and V profiles. The anneals with the different profiles have all been done in a 80x80x350 nm^3 kMC simulation box. The full I, V profiles have been calculated twice, one taking $E_b = 15$ eV as the energy needed to generate a FP in the BCA implant simulator, the other with $E_b = 20$ eV. From Fig. 3 we can conclude again that the original I and V coordinates are not important since the I and V profiles provide a correct anneal simulation. Also, although the damage generated with $E_b = 20$ eV was 20% smaller than for $E_b = 15$ eV the boron spike anneal were the same (not shown in the figure). But the net I and V excess is not enough and the total I and total V concentrations have to be used. This is because the formation of BICs only occurs for very high I concentrations, and then the net I profile is not enough to immobilize the boron spike.

In conclusion, although the present study only deals with a limited range of implant/anneal conditions, it helps clarify which mechanisms of implant simulations can be most relevant for accurate prediction of TED upon a subsequent annealing. To summarize this study (i)FP interstitial and vacancy spatial correlation is not important. (ii) The net I and V excess distributions can yield the correct supersaturation. (iii) Even noisy implant simulations can yield correct results. (iv) Vacancy clusters are not relevant: this reduces the number of equations in I-mediated diffusion modeling in continuum simulators. (v) In simulations with I-mediated diffusion species with clusters (like BICs) it is necessary to use the full I and V profiles, not just the net I and V, because the total particle concentrations are needed to immobilize the impurities in impurity-point defect clusters. (vi) Finally, a practical rule for process simulators is: run a quick, small BCA implant simulation to generate the "noisy" I and V profiles, and use these profiles directly in a large kMC simulation box or use a smooth fit in a continuum simulator.

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