



Strasbourg (France)

MANUSCRIPT COVER PAGE FORM

E-MRS Symposium : B
Paper number : #2000
Title of paper : A kinetic Monte Carlo annealing assessment of the dominant features from ion implant simulations.

Corresponding author : Ignacio Martin-Bragado

Full Mailing Address : Ignacio Martin-Bragado. Dpto. Electronica. Universidad de Valladolid. E.T.S.I.T. Campus Miguel Delibes S/N. 47011. Valladolid. Spain.

Telephone : +34 983 42 30 00 ext 5510
Fax : +34 983 42 36 75
E-mail : ignacio.martin@tel.uva.es

A kinetic Monte Carlo annealing assessment of the dominant features from ion implant simulations

I. Martin-Bragado,* M. Jaraiz, P. Castrillo, R. Pinacho, J.E. Rubio, and J. Barbolla

Dept. de E. y Electronica, Univ. de Valladolid.

ETSIT Campus M. Delibes, 47011 Valladolid, Spain

(Dated: April 30, 2004)

Abstract

Ion implantation and subsequent annealing are essential stages in today's advanced CMOS processing. Although the dopant implanted profile can be accurately predicted by analytical fits calibrated with SIMS profiles, the damage has to be estimated with a Binary Collision Approximation implant simulator. Some models have been proposed, like the “+n”, in an attempt to simplify the anneal simulation. We have used the atomistic kinetic Monte Carlo DADOS to elucidate which are the implant modeling features most relevant in the simulation of transient enhanced diffusion (TED). For the experimental conditions studied we find that the spatial correlation of the I,V Frenkel pairs is not critical in order to yield the correct I supersaturation, that can be simulated just taking into account the net $I - V$ excess distribution. In contrast, to simulate impurity clustering/deactivation when there is an impurity concentration comparable to the net I-V excess, the full I and V profiles have to be used.

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

I. INTRODUCTION

Ion implantation has become the standard process to introduce dopant profiles in CMOS technology, one of the next major challenges for ion-implantation being the fabrication of ultra-shallow source/drain structures. In this process extra interstitials (I) and vacancies (V) are created, which are removed from the device with a subsequent annealing. These annealings cause transient enhance diffusion (TED)[1] which leads to the widening of the implanted profiles. A full understanding on the implant process and subsequent annealing is needed for process simulators to correctly account for TED.

Damage distribution is simulated by process simulators either by means of an analytical approximation or with a binary collision approximation (BCA) code. Part of this damage is due to the implanted ion, which at the end of its trajectory can become substitutional and displace a silicon self interstitial. The other part emerges when the high-energetic ion elastically gives enough energy to the crystalline atoms to break their bonds with the lattice, creating another extra I plus a V . The “+1” model[2] neglects this second contribution assuming that only the ion component will induce TED. This model is based on the assumption that that the Frenkel pair I s and V s recombine locally in the bulk and therefore do not contribute to the enhanced diffusion. In general, the “+1” model needs to be modified to a “+n” model[3, 4] but under certain conditions it has been very successful applied to boron, for example.

II. OUR MODEL

Atomistic kinetic Monte Carlo (kMC) simulations have been used in this study. This simulation method provides a simple and yet exceptionally accurate description of the physical mechanisms involved in micro-electronic processing. It simulates the random walk of each and every diffusing particle in a three dimensional simulation domain, as well as their interactions with the surface or between them to recombine or form extended defects like $\{311\}$ defects, dislocation loops, voids and impurity clusters[5]. 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. We are going to compare TED simulations using these two approaches in order to check the relevance of the

spatial correlation of FPs. We are also going to analyze the relative contribution of the two components of damage, FPs and ion. Another feature that we are going to test is the role of the absolute number of FPs generated by the implanted ion. Finally, we will consider the case of ion implant-induced impurity clustering.

III. SIMULATION RESULTS

In order to study a typical medium-energy, non amorphizing, room temperature implant, we have chosen a 40 keV, $5 \times 10^{13} \text{cm}^{-2}$ Si self implant and a subsequent anneal of 6000 seconds at 738° C, that is enough to recombine all the damage. We use a simulation box with an implant area of $50 \times 50 \text{nm}^2$, which implies the implantation of approximately 1250 ions, and a depth of 350 nm. The cascades are simulated with the BCA implant simulator MARLOWE[6] and the coordinates of I s and V s are transferred to simulate the anneal to the atomistic kinetic Monte Carlo code DADOS[5].

To test the relevance of FP spatial correlation, in Fig. 1 we compare the simulated time evolution of self-interstitial supersaturation from BCA generated particle coordinates, with those using as input the I, V profiles. In the last case, we have translated the concentration profiles back into discrete atoms using a random number generator for in-plane coordinates, so the individual FP spatial correlation is lost. As it can be seen (“FP+Ion” lines in the Figure) there is no noticeable difference, indicating that the IV spatial correlation is not relevant. This validates the use of I, V profiles, which is much faster (using analytic approximations) than generating the cascades with a BCA program. We are also able to analyze the contributions coming from FPs and from the implanted ion (see FP and Ion lines in Fig. 1. As it can be seen, the supersaturation due to the ion is dominant over the one due to FPs, supporting the “+1” model[2] for the simulated conditions.

We have carried out another simulation, Fig. 2, in which the I s and V s are only the net local I or V excess (inset). This new simulation tests the idea that most I s and V s recombine locally, and therefore very fast. The supersaturation produced is the same, corroborating the idea that the number of jumps that the I s perform to recombine locally with V s is negligible. Moreover, the number of net I s and V s is very small compared with their total number, allowing for a less demanding kMC simulation.

Figure 3a shows the total interstitial and vacancy profiles for the previously mentioned

simulation. The full I , V profiles have been calculated three times, one taking $E_b = 15$ eV as the energy needed to generate a FP in the BCA implant simulator (a commonly used value), the others with $E_b = 10$ and $E_b = 20$ eV. As it can be seen in Fig. 3a the different binding energies produce different concentrations of I s and V s, but the $I - V$ net excess is the same (figure 3b) yielding similar supersaturations (figure 3c). This points out that, although E_b may be critical for damage build up simulation, it is not a very sensitive parameter in TED simulations.

A common simplifying assumption in continuum simulators is not to include V clusters, in order to reduce the number of equations. We have verified the validity of this hypothesis by performing simulations with and without the V clusters model. We have verified that the time evolution of the self-interstitial 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.

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[7].

Let us consider now the case of ion implant-induced impurity clustering. As an example we take boron, which is known to react with I s creating BI clusters (BIC) which play a key role in B diffusion and electrical deactivation[8, 9]. We have carried out some simulations to help clarify how the previous conclusions can be affected by the presence of impurities.

Fig. 4 corresponds to the simulated boron profiles of a B spike, after ion implantation and a subsequent annealing. Initially the spike is 20 nm thick and has a concentration of $4.5 \times 10^{19} \text{ cm}^{-3}$. It has been implanted with 40 keV, $9 \times 10^{13} \text{ cm}^{-2}$ Si, and annealed for 50 s at 800° C. We have done the following simulations to test how well different conditions immobilize the boron: (a) reading only the ion, i.e., “+1” model (b) reading the $I - V$ net excess profile, (c) reading the full cascade coordinates and (d) reading the full I , V implant profiles. The simulations have been done in a 80x80x350 nm³ kMC simulation box. As in previous cases the simulation using the full I and V profiles is very similar to the one using defect coordinates from BCA, and both fit very well the experimental results (not shown here)[8]. In contrast, in this case, the simulation using only the net $I - V$ difference or the implanted ion, completely fails to reproduce boron clustering. These simplifying approaches incorrectly predict high boron diffusion and low electrical deactivation. This is because the

nucleation requires a high concentration of interstitials during the first stages of annealing. This concentration is provided by FPs, and it is not enough to use the “+n” or “I-V” models.

IV. CONCLUSIONS

We have studied the effect of I and V correlation in non amorphizing, medium-energy ion implants using BCA in conjunction with an atomistic kMC simulator. The information on FP interstitial and vacancy spatial correlation is not necessary to reproduce the correct I supersaturation. In some conditions the $I - V$ net excess profile can yield the correct supersaturation and therefore, the magnitude of TED. We have also analyzed the different contribution of FPs and implanted ions. Further simulations show that vacancy clusters play only a secondary role, supporting the validity of “+1” model in many cases.

Previous conclusions are only partially valid when there is impurity clustering. In this case the full I and V profiles have to be used to reproduce the clustering mediated diffusion and deactivation: a high concentration of point defects is needed to correctly immobilize impurities.

This work has been partially supported by the Spanish Government under project BFM 2001–2250 and the Castilla y León Regional Government under project VA–010/02.

References

- [1] P. A. Stolk, H. J. Gossmann, D. J. Eaglesham, D. C. Jacobson, C. S. Rafferty, G. H. Gilmer, M. Jaraiz, J. M. Poate, H. S. Luftman, and T. E. Haynes, *J. Appl. Phys.* **81**, 6031 (1997).
- [2] M. Giles, *Journal of the Electrochemical Society* **138**, 1160 (1991).
- [3] L. Pelaz, G. H. Gilmer, M. Jaraiz, S. B. Herner, H.-J. Gossmann, D. J. Eaglesham, G. Hobler, C. S. Rafferty, and J. Barbolla, *App. Phys. Lett.* **73**, 1421 (1998).
- [4] G. Hobler and V. Moroz, in *Simulation of semiconductor processes and devices 2001*, edited by D. Tsoukalas and C. Tsamis (SISPAD, Viena, 2001), pp. 35–37.
- [5] M. Jaraiz, P. Castrillo, R. Pinacho, I. Martin-Bragado, and J. Barbolla, in *Simulation of Semiconductor Processes and Devices 2001*, edited by D. Tsoukalas and C. Tsamis (Simulation of semiconductor processes and devices, SISPAD, Viena, 2001), pp. 10–17.
- [6] M. T. Robinson and I. M. Torrens, *Phys. Rev. B* **9**, 5008 (1974).
- [7] M. Jaraiz, P. Castrillo, R. Pinacho, L. Pelaz, J. Barbolla, G. H. Gilmer, and C. S. Rafferty, in *Si Front-End Processing- Physics and Technology of Dopant-Defect Interactions II*, edited by A. Agarwall, L. Pelaz, H.-H. Vuong, P. Packan, and M. Kase (Mat. Res. Soc., 2000), vol. 610, pp. B11.1.1–B11.1.6.
- [8] L. Pelaz, M. Jaraiz, G. H. Gilmer, H.-J. Gossmann, C. S. Rafferty, D. Eaglesham, and J. M. Poate, *App. Phys. Lett.* **70**, 2285 (1997).
- [9] L. Pelaz, G. H. Gilmer, V. C. Venezia, H.-J. Gossmann, M. Jaraiz, and J. Barbolla, *App. Phys. Lett.* **74**, 2017 (1999).

List of figure captions

FIG 1. Comparison between time evolution interstitial supersaturation using correlated and uncorrelated I and V coordinates. Solid lines has been calculated using coordinates from BCA, while dashed lines has been obtained by in-plain randomization of I and V profiles. The ion component corresponds to the implanted ion (“+1” model), FP to the damage generated by the ion and FP+Ion to the full simulation. Simulation conditions are described in the text.

FIG 2. Interstitial supersaturation time evolution during the annealing at 738°C after a 40 keV , $5 \times 10^{13}\text{ cm}^{-2}$ Si implant. Lines: Reading the BCA implant coordinates. Dashes: generated reading the net $I - V$ profile resulting after the BCA implant and generating uncorrelated coordinates. FP corresponds to the damage generated, without the ion, FP+ion to the full damage. Inset: the resulting net $I - V$ profile for the FP.

FIG 3. a) BCA implant simulation of Si, 40 keV , $5 \times 10^{13}\text{ cm}^{-2}$ with different Si binding energies. b) Net $I - V$ excess concentration generated by the different binding energies. c) The supersaturation produced by the implanted profiles after 6000 s at 738°C are mostly the same.

FIG 4. Simulated profiles of a $4.5 \times 10^{19}\text{ cm}^{-3}$ B spike after 40 keV , $9 \times 10^{13}\text{ cm}^{-2}$ Si implant and 50 s anneal at 800°C . Solid line: BCA ion-only implant. Dashed line: Simulations with only the net $I - V$ profiles. Asterisks: Full BCA implant. Squares: Simulations with full I and V profiles. Notice that the net $I - V$ profiles and the ion-only do not correctly immobilize the B spike.

Figures

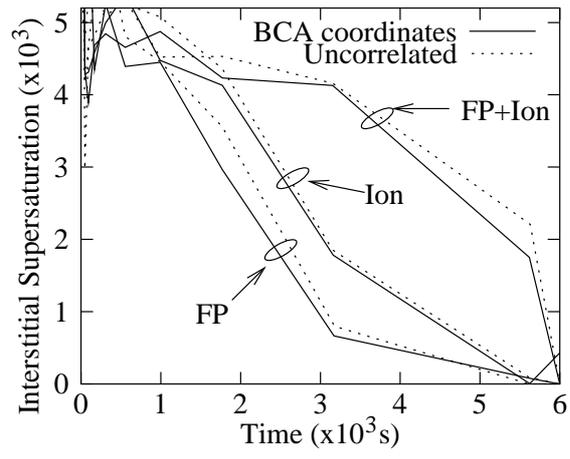


FIG. 1:

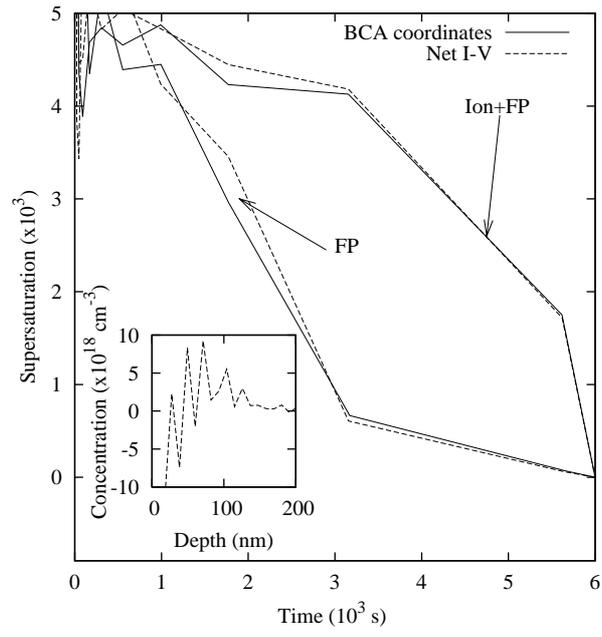


FIG. 2:

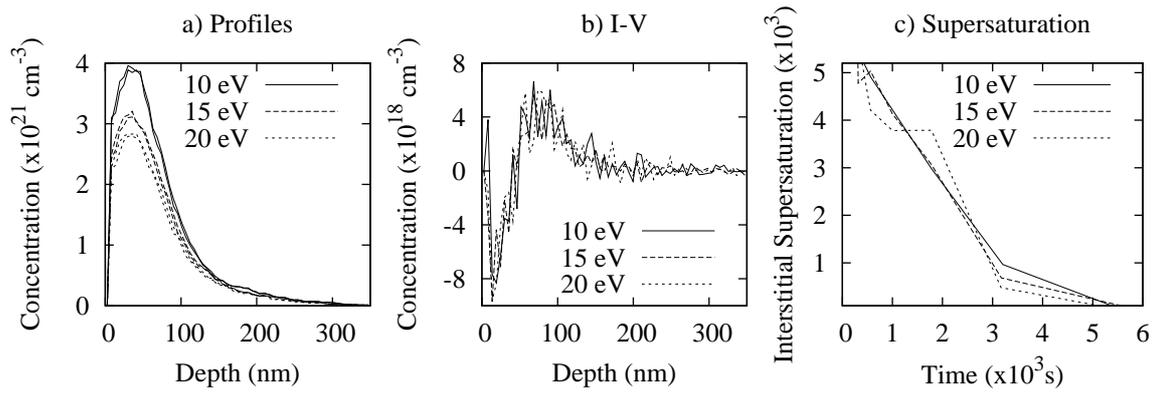


FIG. 3:

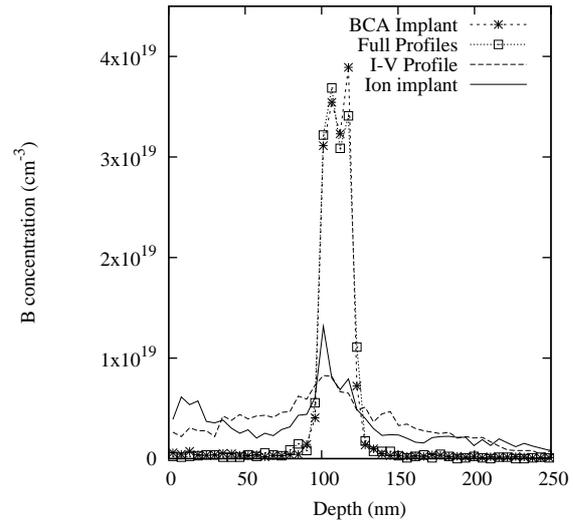


FIG. 4: