Improved atomistic damage generation model for binary collision simulations

Iván Santos,a) Luis A. Marqués, Lourdes Pelaz, and Pedro López

Departamento de Electricidad y Electrónica, E.T.S.I. de Telecomunicación, Universidad de Valladolid, 47011 Valladolid, Spain

(Received 19 January 2009; accepted 26 February 2009; published online 23 April 2009)

We have carried out a classical molecular dynamics study to quantify the conditions under which damage is generated by ion implantation in silicon at energies below the displacement threshold. The obtained results have been used to construct a general framework for damage generation which captures the transition from ballistic (high above the displacement threshold) to thermal (around and below the displacement threshold) regime. The model, implemented in a binary collision code, has been successfully used to simulate monatomic and especially molecular implantations, where nonlinear effects occur. It reproduces the amount and morphology of generated damage at atomic level in good agreement with classical molecular dynamics simulations but with a computational gain factor of \( \sim 10^3 \) to \( \sim 10^4 \). The incorporation of this damage model to process simulators will improve the prediction of amorphization conditions and provide a convenient tool for simulating molecular implants not available to date. Although this work has been focused on silicon, the model can be applied with appropriate calibration to other materials where the thermal regime of damage generation plays an important role. © 2009 American Institute of Physics.

I. INTRODUCTION

Future Si technologies require low resistive ultrashallow junctions as device dimensions are scaled down.1 Low-temperature solid phase epitaxial regrowth (SPER) of amorphous layers has been proposed as a promising technique since it results in a low defect density and a high dopant activation in the recrystallized volume with minimal dopant diffusion.2,3 In the case of \( n \)-type junctions, high-dose As implantation produces self-amorphization of the implanted layer. For \( p \)-type junctions a precrystallizing implant is required when using low-energy monatomic B. However, this B implantation conditions present problems of energy contamination when decelerating the beam due to the existence of neutral B atoms in it. Several B molecules (boron fluoride,4 decaborane,5 and octodecaborane6) have been used to overcome these drawbacks to take advantage of SPER. Nevertheless, after regrowth some defects remain beyond the initial position of the amorphous/crystalline interface and inject Si interstitials during postimplant annealing treatments causing dopant redistribution and deactivation.5,7

It has become of fundamental importance to correctly describe not only the dopant profile but also the generated damage to precisely determine the position of the amorphous/crystalline interface and the amount and morphology of residual damage present after SPER. The small size \( (\sim 10^{-25} \text{ cm}^3) \) and sort lifetime \( (\sim 10^{-11} \text{ s}) \) of the displacement cascades make their experimental characterization very difficult. Theoretical methods that provide an atomistic description of the implantation process are more appropriate for this task. Computer simulation codes based on the binary collision approximation (BCA), such as MARLOWE,8,9 TRIM,10,11 IIS,12 or IMSIL,13 and molecular dynamics (MD) simulation methods14 are two convenient options.

Within BCA, only interactions between the incoming ion and the closest target atom are considered. Two approaches exist to describe the generated damage. The first one is based on the modified Kinchin–Pease (KP) formula.15,16 Models that implement this approach12,17 only follow the ion trajectory and assume that, when a certain amount of energy \( E_{\text{dep}} \) is deposited within a given target volume, the number \( n \) of displaced atoms generated is given by

\[
n = 0.42 \frac{E_{\text{dep}}}{E_d},
\]

\( E_d \) being a constant value that represents the displacement threshold energy of the material. For Si, experimental and theoretical estimations for this energy range from 10 to 30 eV,18–22 but for most simulators it is conventionally taken as 15 eV.9,11,12 When \( n \) exceeds a given percentage of the atomic density within the considered volume, the whole volume is assumed to transform into the amorphous state. In such models ion profiles are obtained in very good agreement with experiments.12 However, the atomic description of damage is lost, and since \( E_d \) is constant they are not able to reproduce nonlinear effects that appear, for example, during the implantation of molecular ions.

Other approach within BCA consists of following not only the trajectory of the ion but also the trajectories of generated recoils, and keeps a full atomistic description of the implantation cascade (“full cascade” BCA).8,11 In this case, a target atom is displaced from its lattice position when it receives in a collision an energy higher than the displacement energy threshold \( E_d \).8 For energy transfers above \( E_d \), the target atom can create a subcascade leaving behind a vacancy.
and generating an interstitial defect where it stops. Thus the generated damage is described in terms of pairs of Si self-interstitials and vacancies, called Frenkel pairs (FP). For energy transfers below $E_d$ no FP are generated and energy is assumed to be lost to phonons. This model adequately reproduces the dilute damage generated by light ions and also give reasonably good depth profiles of implanted species. However, it is not able to reproduce more complex damage structures such as amorphous pockets, which have been observed experimentally after heavy ion implantation. To correctly reproduce the formation of these amorphous pockets, it is necessary to resort to more sophisticated simulation techniques such as MD. This method consists of the numerical resolution of the equations of motion for all the atoms of the simulation cell. Many-body interactions at any energy level (above or below $E_d$) are intrinsically included. However, MD is computationally very expensive and consequently it is limited to relatively small systems and very short simulation times.

The microelectronics industry demands predictive ion-implant atomistic simulators able to correctly describe the damaged structures generated during the implantation but not very computationally demanding. To simulate the complete implantation process at the atomic level, the full cascade BCA approach is usually linked to a kinetic Monte Carlo (kMC) module. The cascade is simulated with BCA, and once it has finished, the coordinates of FP generated are transferred to the kMC module. kMC simulates defect kinetics at the implant temperature considering atomistic models for defect diffusion and interactions, formation and dissolution of clusters and complexes, FP and surface recombination, etc. New cascades are added at time intervals defined by the beam current. This scheme is very convenient because it allows the detailed analysis of the defect evolution during the dynamic annealing step. Postimplant annealing can also be simulated using kMC and complex effects such as the boron anomalous diffusion and the dependence of recrystallization on the particular morphology of amorphous regions can be reproduced.

In order to obtain an adequate description of the generated damage at the atomic level for accurate front-end process modeling, some efforts have been made in the past to accelerate MD calculations for the implantation step. However, introduced approximations in the MD scheme were meant to obtain dopant profiles in very good agreement with experiments but sacrificing the accurate description of lattice damage. Another alternative is the use of multiscale modeling, where several simulation techniques are applied at different time and size scales. One approach consists of linking BCA and MD simulations: evolution of high-energy atoms is simulated with BCA but, when their energy is lower than a certain threshold [500 eV (Ref. 37) or 100 eV (Ref. 38)], MD is used to simulate the final part of the cascade. However, with this approach the most time-consuming stage of the cascade is still simulated with MD, which implies a low computational gain factor. Another alternative consists of using MD simulations to extract mechanisms and parameters that are then fed to BCA simulators.

In this work we have carried out a systematic MD study in order to extract the physical basis of the ion-implant damage generation mechanisms. We have used this information to develop an improved BCA (iBCA) atomistic damage model capable of reproducing amorphous pockets and, in particular, the extensive damage regions generated by molecular implantations. We focus on the energy transfers below $E_d$ that occur during cascades, which are traditionally considered not being employed in the production of atomic displacements. In Sec. II, we describe the MD simulations used to analyze the damage generation mechanisms together with a framework that links the high-energy binary regime with the low-energy thermal regime. In Sec. III, we present the details of the iBCA model. The results applying the iBCA model to monatomic and molecular implantations along with the computational gain factor achieved are described in Sec. IV. Finally, in Sec. V we present the main conclusions of this work.

II. PHYSICAL BASIS OF THE MODEL

During implantation, energetic ions penetrate into the target and lose their energy through collisions with its atoms and electrons. It is traditionally assumed that only energy deposited in the form of nuclear collisions contribute to damage generation, whereas energy transfers to the electronic system are taken as inelastic losses. While energetic atoms are in the ballistic regime (i.e., they have energies well above $E_d$), they can be simulated using BCA. However, as their energy decreases, multiple interactions with target atoms become important. In a previous work we showed using MD that energy transfers among atoms at this low-energy regime can generate amorphous regions. This has also been recently analyzed with ab initio simulations. We explained this damage generation mechanisms as the result of a competition between melting of the lattice and outdiffusion of the deposited energy, in agreement with the traditional concept of thermal spike. To form an amorphous region by this mechanism, it is necessary that the deposited energy remains concentrated locally long enough for melting to be produced before it outdiffuses. We demonstrated that in a Si system where all atoms receive the same amount of energy and dissipation is not possible (due to the periodic boundary conditions), the energy density threshold for amorphization by melting is of just 1 eV/atom. We showed as well that this threshold increases when energy can dissipate, as it happens in real cascades.

A. MD simulations details

All our MD simulations are carried out in the NVE ensemble. Si–Si interactions are described using the Tersoff 3 potential. We use this potential since it gives a very good description of the Si amorphous phase. Besides, it has been successfully used to study the liquid phase of Si and its direct transformation to a-Si upon quenching, the crystal growth from the amorphous phase, and the melt, as well as several phenomena related to ion irradiation in Si. In particular, the evaluation of the displacement energy in Si has resulted in a range of values between 10 and 30 eV (Refs. 19 and 20) in agreement with other experimental and theoretical
values reported. A limitation of this potential is that the predicted crystal melting temperature, 2400 K, is well above the experimental value, 1685 K. However, this is not a serious drawback since it is possible to make a temperature rescaling between Tersoff and real temperatures.

Our simulation cells are cubical and periodic boundary conditions are applied in all directions. Atoms located in a sphere in the center of the cell are given a certain kinetic energy with corresponding velocities in random directions. We will refer to these atoms as initial moving atoms. Their initial kinetic energies are chosen between 0 and 20 eV/atom, around and below the displacement threshold, $E_D$, routinely used in BCA simulators (15 eV). The number of initial moving atoms range from 1 to 100. We also analyze the case of 5000 initial moving atoms to study the trend to the high-energy regime (corresponding to total deposited energies up to 20 keV). In those cases where the number of initial moving atoms is small, we run a total of 100 simulations for each set of initial conditions in order to improve statistics. All simulations are carried out at an initial temperature of 0 K to avoid damage migration and annihilation (we are only interested in damage generation mechanisms since damage annealing is subsequently simulated using KMC). The size of the simulation cell is chosen so that the final temperature increase in the MD cell is not enough to induce damage annealing ($\approx 70$ K). Sizes range from 260 000 to 300 000 atoms depending on the total deposited energy.

To identify damage zones in Si, we use a method based on the time average of atom coordinates, which has been successfully employed to study recrystallization processes in Si and the configurational and energetic properties of the Si self-interstitial. This method consists in performing a time average of atom coordinates over 1000 time steps once the energy of the initial moving atoms is dissipated throughout the cell and thermalization has been reached. This procedure eliminates thermal vibrations and provides the local equilibrium positions for all atoms. During this average there are neither local atomic rearrangements nor changes in the temperature. Then, averaged atomic coordinates are compared with the original perfect lattice positions. When an atom is closer than 0.7 Å to a lattice site the atom is associated with that site; otherwise it is labeled as disordered atom (DA) therefore contributing to damage.

### B. Characterization of damage generation mechanisms

In Fig. 1 we represent the averaged final number of DA in our MD simulations as a function of the initial kinetic energy density for different numbers of initial moving atoms. Contrary to BCA simulations, there is a damage production even for energy densities below 15 eV/atom. This is due to the multiple interactions among atoms, intrinsically included in MD but not considered in BCA simulations. Another interesting aspect that arises from Fig. 1 is that the generated damage strongly depends on the initial conditions: the average final number of disordered atoms increases with the number of initial moving atoms and linearly with the initial kinetic energy density.

Data can be fitted to straight lines given by

$$N_{DA} = \alpha(N)\rho - \beta(N),$$  \hspace{1cm} (2)

where $N_{DA}$ is the final number of DA, $\rho$ is the initial energy density (in eV/atom), and $\alpha(N)$ and $\beta(N)$ are constants for each number of initial moving atoms, $N$. The crossing point of straight lines with the horizontal axis is given by $\beta(N)/\alpha(N)$. This point determines, for each number of initial moving atoms $N$, the minimum initial kinetic energy density necessary to start to promote atoms into a disordered state. For energy densities below this value, it is not possible to permanently perturb the lattice. It therefore represents a threshold energy density for damage production, $E_T$. In Fig. 2 we represent the parameter $E_T(N) = \beta(N)/\alpha(N)$ as a function

![Figure 1](image1.png)

**FIG. 1.** (Color online) Final number of DA in the MD simulations as a function of the initial kinetic energy density for different numbers of initial moving atoms. The straight dashed lines correspond to linear fits of the data.

![Figure 2](image2.png)

**FIG. 2.** Threshold energy density, $E_T$ (circles in top figure), and damage generation cost, $D_C$ (circles in bottom figure), as a function of the number of initial moving atoms $N$ obtained from the straight lines of Fig. 1 (bottom axis). The solid lines correspond to $E_T$ and $D_C$ as a function of the number of energetic local neighbors $N_{LN}$ (top axis). See Sec. III for details.
of the number of initial moving atoms $N$. It decreases when $N$ increases and tends to 1 eV/atom as $N$ goes to infinity. This lower limit agrees with the minimum energy density value necessary to totally melt samples in which all the atoms receive energy, i.e., when $N \rightarrow \infty$, and there is not energy out-diffusion to surrounding regions. The slope of straight lines of Fig. 1, $\alpha(N)$, informs about the damage production yield. We define the damage generation cost, $D_C$, as $D_C(N) = N/\alpha(N)$ (in eV/atom), which is also represented in Fig. 2. It also decreases with $N$ but tends to 0 as $N$ goes to infinity, because when all the atoms receive energy which cannot dissipate, apart from melting it is not necessary any additional energy to reach the final disordered state in the whole cell.

Taking into account the definitions of $E_T(N)$ and $D_C(N)$, Eq. (2) can be rewritten as

$$N_{\text{DA}} = \frac{N \cdot \rho - N \cdot E_T(N)}{D_C(N)}.$$  \hspace{1cm} (3)

This expression is formally similar to the modified KP formula given by Eq. (1), where according to the previous discussion $N \cdot \rho$ is the deposited energy ($E_{\text{dep}}$), and $D_C$ plays a similar role to $E_d/0.42$. Nevertheless, Eq. (3) implies that in order to generate damage, it is necessary first to overcome an energy threshold, given by $N \cdot E_T$, in order to reach an initial disordered estate. The surrounding crystal lattice may force disordered atoms to come back to perfect lattice positions. In order to keep atoms permanently disordered, or at least a fraction of them, an additional amount of energy is required. $D_C$ therefore controls the final number of DA that are generated with the remaining energy. As $N$ increases both $E_T$ and $D_C$ decrease, because it is easier to remove an atom from its perfect lattice position and keep it disordered when its neighboring atoms are also energetically excited.

Note that the energy density required to disorder all the initial moving atoms is given by $\rho(N_{\text{DA}}) = E_T(N) + D_C(N)$, i.e., it is the sum of the corresponding threshold energy density and the damage production cost. In the case of only one initial moving atom ($N=1$), the energy needed to permanently displace it from its perfect lattice position is equal to $\sim 10+ \sim 12=22$ eV, which lies in the range of experimental and theoretical estimations for the traditional displacement energy value in silicon (10–30 eV). In the limit case of $N \rightarrow \infty$, we have a lower limit of $1+0 = 1$ eV/atom, which corresponds to the melting process. Consequently, the transition in damage generation mechanisms between ballistic and thermal regimes is naturally included in the dependence of both $E_T$ and $D_C$ with $N$.

III. IBCA DAMAGE MODEL

In order to efficiently implement in a computer code the ideas described in Sec. II, we will define the iBCA as a local atomistic model by focusing on each atom and its neighbors. Considering the Si density, we have estimated that each atom can be surrounded by up to 26 neighbors (in a cubic volume defined by the second neighbor distance, 3.84 Å, on each direction around the selected atom, as it is also considered in kMC simulators). As we have shown, damage production is highly influenced by energy deposition conditions, i.e., the initial number of atoms that receive energy and the energy density. In our MD simulations, we have only considered cases where the excited region is spherical and the initial energy is the same for all the atoms. However, in real cascades both the geometry and the energy per atom may be quite different. In a local atomistic model, the particular geometry of the simulated cascade will naturally be accounted for. With respect to energy, we showed in a previous work that the initial energy distribution does not influence damage generation noticeably since it is rapidly redistributed among the moving atoms long before damage generation takes place. Consequently, we will consider the average kinetic energy of the local atomic environment to evaluate the final damage. Only surrounding atoms with an energy of 1 eV or above will be taken into account since, as it was mentioned before, below this energy density no DA are produced.

We have defined the damage generation efficiency, $\text{eff}$, as the number of disordered atoms per initial moving atom. It is obtained from Eq. (3) as

$$\text{eff} = \frac{N_{\text{DA}}}{N} = \frac{\rho - E_T}{D_C},$$ \hspace{1cm} (4)

where $\rho$ is the energy density. If we want to apply this expression within a local atomistic model, $\rho$ should represent the average energy density only in the surrounding environment. Analogously, $E_T$ and $D_C$ should be redefined in terms of local energetic neighbors, $N_{\text{LN}}$ (number of local neighbors with energies of 1 eV or above). For that purpose we have evaluated the average number of energetic neighbors of the initial moving atoms in our MD simulations. The solid lines in Fig. 2 represent the resulting dependence of $E_T(N_{\text{LN}})$ and $D_C(N_{\text{LN}})$. The slope of straight lines in Fig. 2 represent the resulting dependence of $E_T(N_{\text{LN}})$ and $D_C(N_{\text{LN}})$. Best fits are given by

$$E_T(N_{\text{LN}}) = 11.348(N_{\text{LN}} + 1)^{-0.837} + 0.931,$$  \hspace{1.5cm} (5)

$$D_C(N_{\text{LN}}) = 11.211 \exp(-0.146N_{\text{LN}} + 0.001 58N_{\text{LN}}^2).$$ \hspace{1.5cm} (6)

In these expressions $E_T(N_{\text{LN}})$ and $D_C(N_{\text{LN}})$ retain most of the features of the original values of Fig. 2. The energy required to generate 1 DA from one initial moving atom (which has 0 local energetic neighbors) is $\sim 22$ eV. On the other hand, the threshold energy density for the damage generation still has the lower limit around 1 eV/atom (atoms in the core of an energetic region will have their environment full of energetic neighbors).

The procedure followed in our iBCA model is represented in Fig. 3. The collisional phase of the cascade is simulated with a conventional BCA code. The BCA simulator provides the position of the FPs generated during the cascade, the remaining energy of the recoils at the end of their trajectories, the position of all the atoms that receive any amount of energy during the cascade (we will call them hot particles), and the amount of energy they receive. Then, at the end of the collisional phase we have a set of vacancies, interstitials, and hot particles.

Within BCA, the energy conservation principle applied to elastic binary collisions implies that the energy of the incident particle must be equal to its energy after the collision plus the recoil energy plus the energy required to take
the recoil away from its lattice site \( (E_d) \). A moving atom is stopped when its energy is not enough to generate more subcascades. However, the remaining energy of the generated interstitial at the end of its trajectory can still contribute to generate more damage if low-energy interactions were modeled. In order to consider this effect within the iBCA model, the residual energy of each generated interstitial is equally shared with its neighboring atoms. High energy interactions only consider the impinging atom and the closest target atom (two-body interactions), but as energy decreases collisions with several target atoms occur more often and groups of energetic atoms are created as the cascade develops (many-body interactions). In that situation the atomic movements will make easier the recoil generation and therefore the creation of vacancies. In order to take into account this effect within iBCA, we have considered that vacancy generation is also environment dependent and controlled by \( D_v \). At each point where a vacancy has been generated, the difference between \( E_d \) (energy to generate FP in binary collisions) and the corresponding value of \( D_v \) (energy cost to displace atoms within an excited neighborhood) according to the local environment is equally shared with the neighboring atoms. In all cases we have chosen a second neighbor distance to share the energy.

After this energy rearrangement, we evaluate which atoms are disordered taking into account their efficiencies from Eq. (4). If the calculated efficiency of a given atom is below zero, it is not disordered. When it is between 0 and 1, the atom is disordered with a random probability given by its efficiency. When it is 1 or above, the atom is disordered and a random neighbor is disordered or not taking into account the remaining efficiency \( (\text{eff} - 1) \), and so on. In order to simulate the energy diffusion process, we first evaluate the efficiency of those atoms with the highest amount of energy on their environment, and the process is repeated until no further energy remains to create more disordered atoms. Finally, we consider additional disordering of atoms taking into account the local distortion of the lattice. It would not be reasonable to consider that an atom surrounded by disordered atoms is not disordered itself. Consequently, once we have applied the efficiencies, we search for nondisordered atoms that have more than half of their nearest neighbors disordered.

It is worth to note that this scheme for damage generation can be regarded as a combination of the two traditional BCA approaches for damage description. As in full cascade BCA, ion and recoil trajectories are followed to generate damage at the atomic level and provide the individual position of FP, but we also consider the energy deposited in atoms not displaced by ballistic collisions. This energy is used to generate thermally disordered atoms following a scheme similar to the modified KP approach. Nevertheless, since the residual deposited energies we are considering to determine efficiencies are always at the low-energy regime, we guarantee the local character of damage generation. In addition, expression (3) accounts for phase transformation (melting) and heat dissipation through the dependence of the parameters \( E_T \) and \( D_v \) on the number of energetic neighbors. This feature captures the nonlinear effects on damage generation due to the proximity of several energetic atoms as it occurs in molecular implants.

**IV. RESULTS OF IONIC IMPLANTATION**

In this section we present the results of applying the iBCA model to reproduce the damage generated during monatomic and molecular implantations into Si. We show as well the computational efficiency of our model in comparison with MD.

**A. Monatomic implantation**

We have simulated iBCA independent cascades of B, Si, and Ge into Si(100) at 0 K with a tilt of \( 7^\circ \) to avoid channeling. Implantation energy is chosen so that the nuclear deposited energy is 1 keV in all cases. Since damage is assumed to be generated by nuclear collisions, the nuclear deposited energy can be used as a reference value to compare the damage generated by different ions. In order to make a statistical study, we have carried out 200 iBCA cascades for each ion. These simulations are compared with equivalent MD simulations, i.e., cascades of B, Si, and Ge into Si with 1 keV of nuclear deposited energy.

Table I summarizes the obtained results. In conventional BCA the number of FP generated during a cascade only depends on the amount of nuclear deposited energy. Then, different ions implanted with the same nuclear deposited energy generate the same number of FP. However, it has been observed through experiments and MD simulations that heavier ions produce extensive defects and amorphize the target easily. With our model we are able to capture this increase in generated damage with ion mass obtaining an average number of DA similar to the observed in MD simulations. In addition, when we group these DA within a first neighbor distance to find clusters of defects, average mean and maximum cluster sizes are close to MD results. Furthermore, as ion mass increases, the percentage of DA in big clusters increases while the percentage in small clusters decreases, trend which has also been observed in MD.
TABLE I. Summary of the results obtained for cascades of B, Si, and Ge into Si with 1 keV of nuclear deposited energy using conventional BCA, MD (Ref. 57), and iBCA. The average numbers of FP (conventional BCA) and DA (MD and iBCA) are shown. We also show for MD and iBCA the average mean and maximum cluster sizes and the percentages of DA in clusters of different sizes.

<table>
<thead>
<tr>
<th></th>
<th>B</th>
<th>Si</th>
<th>Ge</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conventional BCA</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Average number of FP</td>
<td>15</td>
<td>17</td>
<td>16</td>
</tr>
<tr>
<td>MD</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Average number of DA</td>
<td>68</td>
<td>89</td>
<td>130</td>
</tr>
<tr>
<td>Mean cluster size</td>
<td>8.6</td>
<td>22.2</td>
<td>63.5</td>
</tr>
<tr>
<td>Mean maximum cluster size</td>
<td>14.9</td>
<td>32.2</td>
<td>80.9</td>
</tr>
<tr>
<td>Distribution of DA in clusters (%)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Size ≤ 10</td>
<td>83.4</td>
<td>58.6</td>
<td>32.1</td>
</tr>
<tr>
<td>10 &lt; Size ≤ 50</td>
<td>14.9</td>
<td>29.2</td>
<td>16.7</td>
</tr>
<tr>
<td>Size &gt; 50</td>
<td>1.7</td>
<td>12.2</td>
<td>51.2</td>
</tr>
<tr>
<td>iBCA</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Average number of DA</td>
<td>61</td>
<td>77</td>
<td>124</td>
</tr>
<tr>
<td>Mean cluster size</td>
<td>9.3</td>
<td>17.5</td>
<td>72.2</td>
</tr>
<tr>
<td>Mean maximum cluster size</td>
<td>17.3</td>
<td>29.2</td>
<td>90.9</td>
</tr>
<tr>
<td>Distribution of DA in clusters (%)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Size ≤ 10</td>
<td>63.3</td>
<td>45.9</td>
<td>17.2</td>
</tr>
<tr>
<td>10 &lt; size ≤ 50</td>
<td>33.6</td>
<td>43.8</td>
<td>12.6</td>
</tr>
<tr>
<td>Size &gt; 50</td>
<td>3.1</td>
<td>10.3</td>
<td>70.2</td>
</tr>
</tbody>
</table>

Differences in these percentages between MD and iBCA arise from the fact that small defect clusters can have different configurations with different numbers of DA. For example, the Si self-interstitial can be in one of the several possible configurations: in the so-called “extended” configuration it consists of four DA, while in the “tetrahedral” configuration only one atom is disordered with respect to the perfect lattice. These different configurations that appear in MD but not in iBCA increase the percentage of DA in small clusters and also the final number of DA in MD simulations with respect to iBCA.

Note that even for light ions, the final damage is highly increased (from 15 FP to 68 DA for B). Nevertheless, in this case DA belonging to small clusters will recombine easily even at room temperature. In the case of Ge, we obtain a higher increase, i.e., the effect of low-energy interactions is more important for heavy ions. In addition, generated DA belong to bigger clusters that have a higher probability of surviving, therefore contributing to damage accumulation and thus substrate amorphization.

The percentage of cascades that produce a given number of FP (conventional BCA) or DA (MD and iBCA) is represented in Fig. 4. Distributions shown are almost equal for the three ions with conventional BCA, which is not the case for MD. However, the iBCA model provides a distribution very similar to MD. Therefore, our improved damage model does not only give a damage description in better agreement with MD, but it also reproduces its atomistic morphological characteristics.

B. Molecular implantation

Although molecular implants are becoming more and more relevant in the fabrication of microelectronic devices, current atomistic process simulators do not have the capability of simulating them. MD calculations have revealed that molecular implantations generate highly damaged regions in the Si substrate due to the ion-induced melting. However, MD is too slow to be used routinely in process simulations and, on the other hand, these amorphous regions cannot be reproduced just with the superposition of conventional BCA monatomic B cascades. Our iBCA model provides a solution to this problem.

We have simulated the implantation of octadecaborane into silicon using iBCA. For the sake of simplicity, and to compare with previous MD results, we have only considered the B atoms in the molecule. To make a statistical study we have carried out 100 independent cascades of 9 keV $\text{B}_{18}$ into Si with normal incidence (500 eV per B atom). Electronic stopping power was evaluated using the Brandt–Kitagawa modified stopping model. We have simulated a sequential monatomic implantation of 18 B ions using BCA, and we store the set of FP and hot particles generated by each ion. At the end of the sequential implantation, we consider simultaneously all the generated particles for the dam-
age generation iteration within iBCA. The impact point of each ion is randomly chosen within a square implantation window, its sides being equal to the diagonal of the octadecaborane molecule.

In the iBCA model, the average number of disordered atoms generated per boron ion is $108 \pm 9$ (1946 $\pm 153$ in total), while it is only $28 \pm 8$ per monatomic B implantation and $7 \pm 2$ FP for conventional BCA. Consequently, there is a great enhancement in damage production when implanting the molecule. Furthermore, the rate of damage generated per ion in the molecular implantation compared to the monatomic implantation is in very good agreement with the MD results. In order to illustrate the difference between conventional BCA and iBCA, we have represented in Fig. 5 the damage generated by a $\text{B}_{18}$ cascade. Conventional BCA only provides the position of the implanted ions and the generated Si interstitials and vacancies. However, iBCA also provides the position of the additional DA generated after applying the efficiencies. As it can be seen, a large number of DA surround the cascade area. In the case of MD simulations, amorphous zones show an average diameter of 4 nm from the surface to a depth of 3 nm, and conical from 3 nm to around 5 nm below the surface, results comparable with those obtained with our improved damage model.

C. Computing time reduction

In Table II, we have summarized the average simulation times required for the calculations described in Secs. IV A and IV B for MD and iBCA. We also show the time gain factor of iBCA with respect to MD. All simulations were carried out in a 3 GHz Pentium IV processor. As it can be seen, simulation times decrease for monatomic implantations as ion mass increases in both MD and iBCA. This is due to the fact that light ions penetrate deeper in the target for the same implantation energy, and consequently bigger simulation cells are needed both in MD and iBCA to encompass the full implantation cascade. On the other hand, computational times are longer for molecular ions than for monatomic implantations in all cases. Longer computational times are needed because the cascade generated by the molecular ion is bigger, and more time steps are required until the deposited energy is fully dissipated throughout the target. Furthermore, the number of particles that conventional BCA provides to the damage generation algorithm of iBCA is bigger. Nevertheless, the gain factor of iBCA with respect to MD ranges from $\sim 2000$ for molecular implants to $\sim 8000$ for Ge implantation, i.e., iBCA is three to four orders of magnitude faster than MD while providing the same damage description.

V. CONCLUSIONS

By using MD simulation techniques, we have developed an atomistic model for the description of ion-implant damage generation mechanisms in Si. The model is based on the environment conditions in which energy is locally deposited in the target by considering all energy transfers included those below the displacement threshold, contrary to conventional BCA. We have described the damage generation process in terms of the energy density threshold $E_T$, which determines the minimum energy density necessary to reach a metastable disordered state, and the damage generation cost $D_C$, which defines the fraction of atoms that stay permanently disordered. The dependence of these two parameters with the number of energetic local neighbors accounts for the transition in damage production between ballistic and thermal regimes. Furthermore, this dependence captures nonlinear effects on damage generation clearly manifested in molecular implants can be described.

It is important to note that while our iBCA model takes into account the dissipation of energy throughout the target no heat diffusion equation needs to be solved. Furthermore, the model has few parameters with a clear physical interpretation, and thanks to its local description it can be used to simulate different implantation conditions with no additional fitting when ion species or implant energy are changed. It has been successfully applied to simulate monatomic and molecular implantations into Si. It correctly predicts the formation of amorphous regions for the case of heavy and molecular ions, in very good agreement with the MD results, as well as the dependence of the amount and morphology of damage with ion mass (where conventional BCA fails). Simulations using iBCA are between three and four orders of magnitude faster than equivalent MD calculations.

In summary, our iBCA model provides an atomistic description of damage much better than conventional BCA in a reasonable computational time. The incorporation of iBCA to process simulators will allow the accurate prediction of
amorphization conditions, as well as providing a convenient tool for the simulation of molecular implants not available to date. Although this work has been focused on Si, the iBCA model can be applied with appropriate calibration to other materials and technological processes where ion implantation plays an important role.

ACKNOWLEDGMENTS

This work has been supported by the Spanish DGI under Project No. TEC2008-06069.

23In the MD simulations presented in Sec. II B, we have found that, for the energy deposition conditions found in implantation cascades, disordered atoms are not further than the second neighbor distance with respect to the border of the sphere of the initial moving atoms. This limit can be taken as the influence distance of multiple-interactions for damage generation at this energy regime.
47In the MD simulations presented in Sec. II B, we have found that, for the energy deposition conditions found in implantation cascades, disordered atoms are not further than the second neighbor distance with respect to the border of the sphere of the initial moving atoms. This limit can be taken as the influence distance of multiple-interactions for damage generation at this energy regime.