Atomistic Simulation Techniques in Front-End Processing

Luis A. Marqués, Lourdes Pelaz, Iván Santos, Pedro López, and María Aboy
Department of Electronics, University of Valladolid, ETSI Telecomunicación, Campus Miguel Delibes s/n, Valladolid, 47011, Spain

ABSTRACT

Atomistic process models are beginning to play an important role as direct simulation approaches for front-end processes and materials, and also as a pathway to improve continuum modeling. Detailed insight into the underlying physics using \textit{ab-initio} methods and classical molecular dynamics simulations will be needed for understanding the kinetics of reduced thermal budget processes and the role of impurities. However, the limited sizes and time scales accessible for detailed atomistic techniques usually lead to the difficult task of relating the information obtained from simulations to experimental data. The solution consists of the use of a hierarchical simulation scheme: more fundamental techniques are employed to extract parameters and models that are then feed into less detailed simulators which allow direct comparison with experiments. This scheme will be illustrated with the atomistic modeling of the ion-beam induced amorphization and recrystallization of silicon. The model is based on the bond defect or IV pair, which is used as the building block of the amorphous phase. It is shown that the recombination of this defect depends on the surrounding bond defects, which accounts for the cooperative nature of the amorphization and recrystallization processes. The implementation of this model in a kinetic Monte Carlo code allows extracting data directly comparable with experiments.

INTRODUCTION

Silicon processing is facing an increasingly high level of complexity as CMOS technology is pushed closer to its limits. In particular, front-end processing is trying to extend the use of conventional and well established techniques, such as ion implantation and annealing, into the nanometer regime [1]. With further reduction of the devices size, new effects or effects that were neglected so far become relevant. Their experimental characterization is a complex task, firstly because the realization of test lots is extremely expensive, and secondly because usually these effects occur simultaneously which makes difficult the interpretation of measurements. In this situation the use of simulation tools can be very helpful [2].

Most process simulators used in industrial applications are based on continuum methods, where the physics of the system is formulated as a series of differential equations for each particle type considered to be relevant in the process. Typically they are continuity equations, where each particle gain or loss is formulated in terms of its generation and recombination rates and the diffusion flux [3,4]. In the equations there are a number of parameters such as binding energies, diffusivities, capture radii, etc., that have to be provided. The numerical solution of the set of partial differential equations requires spatial and temporal discretization. Continuum simulators are fast and allow the consideration of big sample sizes by adjusting the grid used for the spatial discretization. However, this advantage is reduced as the device size shrinks to nanometric scale. The atomistic nature of the material arises and complex physical interactions show up. The use of a very refined grid and the addition of new equations slow down the resolution of the problem using continuum methods. Then atomistic simulation techniques become a good alternative even for industrial applications [5].
In this paper we show how atomistic simulation techniques can be used to get physical insight on some of the aspects related to the front-end processing of Si. In particular, we will focus on the modeling of the ion-beam induced amorphization and subsequent recrystallization of the Si substrate, which has been defined as a key challenge in the successive editions of the International Technology Roadmap for Semiconductors [2].

ATOMISTIC SIMULATION TECHNIQUES

In atomistic simulation methods the system under study is described as a set of interacting particles. Depending on the accuracy used to describe the interactions it is possible to distinguish several techniques. In the so-called *ab-initio* methods, the Schrödinger equation is solved for the set of nuclei and electrons which constitute the system under study. They provide an accurate description of the interactions based on the electron distribution of the atoms, with no parameters [6-9]. However, these methods are computationally very expensive, and thus they can only handle systems of a few hundred atoms and are limited to extremely short times. On the other hand, classical molecular dynamics (MD) simulations describe atomic interactions by empirical force laws which include several parameters chosen by fitting to experimental data or *ab-initio* calculations [10,11]. It is possible to simulate systems containing millions of atoms for times of the order of nanoseconds, but at the expense of losing the electronic description of the system [12,13]. The *tight-binding* (TB) technique, based on the method of linear combination of atomic orbitals [14], is an alternative half-way between *ab-initio* and classical MD. It is a non-parameter-free approximation [15] that allows the use of intermediate sizes and times while keeping the electronic description of the system. In summary, these simulation methods allow a full description of the system dynamics at the atomic level. However, they are computationally expensive techniques, and size and time scales accessible to them are still orders of magnitude far from actual processing scales.

In order to bridge the gap between these detailed atomistic techniques and experiments several simulation methods can be used. These methods maintain the atomic-level description, but in order to reach experimental scales they must renounce to keep the full dynamics of the system. In the so-called *binary collision approximation* (BCA) the implantation process is simulated by calculating collisions between energetic atoms and target atoms by assuming that they interact in pairs [16]. Thousands of cascades can be easily calculated to give enough statistical resolution in the generation of dopant profiles. However, damage profiles in amorphizing conditions are not so well predicted, precisely because multiple interactions are not taken into account in the calculation. On the other hand, *kinetic Monte Carlo* (kMC) codes allow the simulation of the annealing step [1-5]. Unlike MD, the vibrational movement of the Si lattice atoms is not simulated, only the dynamics of defects and dopants is followed, which allows the simulation of system sizes typical of today’s devices. Parameters that define the dynamics of defects, such as diffusivities, binding energies, capture radii, etc., must be specified. The simulation time-step is variable. It may go from $10^{-9}$ s for the diffusion of point defects to $10^{-3}$ s, or even longer, for the emission of defects from stable clusters. Generally fast events tend to disappear quickly leaving slower events that raise the time-step. This allows to easily access macroscopic times, and so to the simulation of actual processing.

No individual technique can be used alone for the simulation of full Si processing. Each one gives information at a different scale level, so all of them have to be used in a hierarchical or
multi-scale scheme. Fundamental techniques such as *ab-initio* and TB can be employed to study defect configurations and energetics, material and electronic properties, and to optimize empirical force potentials along with experimental data. Classical MD in turn can be used to determine interaction and diffusion mechanisms involving defects, or to study the damage morphology obtained from individual implantation cascades as well as its annealing behavior. All these data along with experimental measurements will define the relevant events to be considered in the kMC simulator. The BCA code is used to calculate the implantation cascades. The coordinates of dopants and generated defects are fed to the kMC simulator at time intervals determined by the dose-rate. This procedure is repeated until the specified dose is reached. Afterwards, subsequent anneals can be also simulated.

In the next sections we will show how to apply this hierarchical simulation scheme to develop an atomistic model for the ion-beam induced amorphization and subsequent recrystallization of Si, processes of technological relevance.

**MODELING DAMAGE GENERATION**

As it has been already mentioned, implantation is usually simulated using BCA codes, by calculating collisions between the ion and its closest target atom. A target atom is displaced from its position when it receives in a collision an energy higher than the displacement threshold, $E_d$, conventionally 15 eV for Si [17,18]. In that situation, the target atom can become a recoil leaving behind a vacancy and creating a subcascade. For energy transfers below $E_d$ no recoiling atoms are formed and energy is assumed to be lost to phonons [19]. Then, BCA describes damage in terms of these created interstitial-vacancy pairs, also called *Frenkel Pairs* (FP). In turn, MD simulations naturally take into account multiple interactions among atoms, and all energy transfers can contribute to possible displacement events. Damage is described in terms of atoms displaced from perfect lattice positions and the corresponding empty lattice sites.

Figure 1 represents the percentage of cascades producing a certain number of FP for BCA and displaced atoms for MD in 1 keV implants of B, Si and Ge ions into Si. BCA produces the same average number of Frenkel pairs and distributions are very similar. However, in MD the amount of damage increases with ion mass, in agreement with experiments [20].

![Figure 1](image-url)

*Figure 1*. Percentage of cascades generating a certain number of FP in BCA and displaced atoms in MD for 1 keV B, Si and Ge cascades into Si. Average numbers of FP and displaced atoms created by each ion are also shown.
In a more detailed analysis of energy transfers in BCA during the cascade, we find that only 23% of deposited energy is used to generate Frenkel pairs (see Table I). The remaining percentage, 77%, is not employed in displacement processes but in energy transfers to atoms below the threshold. If we group them within a first neighbor distance, we find that mean group size and mean group energy increases with ion mass. Consequently, it seems that these low energy transfers usually ignored in BCA simulations could establish the difference in damage morphology between the three ions.

**Table I.** Average results obtained from BCA simulations of 1 keV B, Si and Ge implantations into Si: percentages of deposited energy employed in the generation of FP and in energy transfers below $Ed$, mean size and mean energy of groups of target atoms which receive energies below $Ed$.

<table>
<thead>
<tr>
<th></th>
<th>FP</th>
<th>BELOW $Ed$</th>
<th>MEAN SIZE</th>
<th>MEAN ENERGY (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>22.0 %</td>
<td>78.0 %</td>
<td>15.2</td>
<td>92.4</td>
</tr>
<tr>
<td>Si</td>
<td>23.3 %</td>
<td>77.7 %</td>
<td>29.6</td>
<td>180.8</td>
</tr>
<tr>
<td>Ge</td>
<td>24.0 %</td>
<td>76.0 %</td>
<td>50.5</td>
<td>311.4</td>
</tr>
</tbody>
</table>

Our aim is to develop an improved BCA model able to provide a description of damage equivalent to the prediction given by MD calculations. For that purpose, we have carried out MD simulations to study the damage generation processes at energy transfers below the displacement threshold [21,22]. We give a certain amount of kinetic energy to a number of atoms located in a sphere in the center of the simulation cell with velocities in random directions. The initial energy of moving atoms varies between 0 and 20 eV per atom, around and below the displacement threshold for Si, and the total deposited energy between 50 and 500 eV, of the order of energies found in BCA simulations. We define the efficiency of damage production as the number of final displaced atoms per initial moving atom.

Figure 2 shows the obtained efficiency of damage production as a function of the initial energy of moving atoms for different total deposited energies. In BCA simulations, the efficiency is zero below the displacement threshold and one over it. However, in MD the efficiency can be quite high even below the threshold. This efficiency increases with initial energy of moving atoms and with the total deposited energy. As it can be seen, the same amount of deposited energy is more or less efficient in terms of damage generation depending on the energy density. When this is high, deposited energy remains concentrated long enough to promote local amorphization.

We have used these MD results to incorporate the effect of low energy interactions in BCA models. The first step is to consider all energy transfers to target atoms, and not only those above the threshold. Then we group these atoms within a first neighbor distance. Taking into account the number of particles and total energy of the formed groups, we apply the corresponding efficiency to obtain the amorphous regions. As shown in Table I, formed groups in BCA cascades of 1 keV B had mean energies around 100 eV, and the average energy per atom was 6.1 eV. Then the corresponding efficiencies are around 0.5. Analogously, Si groups have efficiencies around 0.8 and Ge groups around 1.2. This means that in Ge damage production due to low-energy interactions is more efficient.
Figure 2. Efficiency of damage production as a function of the initial energy of moving atoms for different total deposited energies. Dashed line represents the efficiency of BCA simulations.

We have applied this model to the simulations described in figure 1 and table I. Figure 3 represents the distributions of cascades as a function of the amount of generated damage within this improved BCA model. The average number of displaced atoms for each ion is also shown. In the improved BCA, we can see that now ions produce different number of displaced atoms, with a distribution very similar to that obtained with MD and shown in figure 1 [20].

Figure 3. Percentage of cascades generating a certain number of displaced atoms obtained from simulations of 1 keV B, Si and Ge implants into Si using the improved BCA model. Average numbers of displaced atoms are also shown.

MODELING THE AMORPHOUS PHASE

In order to simulate amorphization and recrystallization processes at the atomic level in Si it is essential to identify the defect that can be used to describe the amorphous phase. We have
based our atomistic model in the bond defect. Its atomic structure is shown in figure 4. It consists of a local rearrangement of bonds in the crystal with no excess or deficit of atoms. As it can be seen, it introduces in the Si lattice the five- and seven-membered rings typical of the amorphous phase while maintaining perfect four-fold coordination.

Figure 4. Atomic structure of the bond defect. Dashed lines represent atoms and bonds in the perfect lattice. Atoms A and A' move along the directions indicated by the arrows and switch their bonds with atoms B and B', giving rise to the bond defect.

Tang and coworkers encountered the bond defect when studying self-diffusion and interstitial-vacancy recombination in Si using TB techniques [23]. They found that when a vacancy approaches a dumbbell interstitial, a metastable defect structure is generated instead of having immediate interstitial-vacancy recombination. For this reason the bond defect is also known as IV pair. Using classical MD techniques, Stock and coworkers observed that the bond defect can be also generated as a result of a pure ballistic process [24]. Thus the IV pair can be a primary defect generated by irradiation, with no need of pre-existing interstitials and vacancies in the lattice for its formation. Information regarding the structure and energetics of this defect has been extracted using ab-initio, TB and classical MD techniques [23,25-27]. One of the most important parameters to determine in order to study the role of the IV pair in the amorphization process is its stability. It has been shown using classical MD that its lifetime follows an Arrhenius behavior with an activation energy of 0.43 eV [27]. At room temperature, the IV pair lifetime is about 3 μs, very short in comparison with the characteristic inter-cascade time at typical dose-rates. This indicates that the IV pair as an individual defect is not stable enough to accumulate and promote amorphization.

However, the stability of the IV pair increases when other IV pairs are present in the lattice [27]. In figure 5 we show the time evolution at high temperature of the mean potential energy per atom in crystal lattices where several concentrations of IV pairs were introduced. Atomic energy levels corresponding to a full amorphous matrix, $E_{AM}$, and to a perfect crystal, $E_{C}$, are also shown. For an initial concentration of 30% the mean potential energy decreases only to the amorphous level. In fact, the obtained structure is identical to a pure amorphous matrix. On the other hand, in lattices with starting concentrations of 10, 20 and 25% full recrystallization occurred. In the case of 10%, the evolution is exponential, with a decay time similar to the lifetime of an isolated IV pair at the same temperature. Thus 10% is a concentration so low that IV pairs do not interact strongly with each other. They recombine one by one, and the overall crystallization behavior is the same as when you have just one IV pair. On the other hand, for higher concentrations the evolution of the potential energy per atom shows plateaus followed by steps, indicated by arrows. This behavior has been also observed in experiments on the recrystallization kinetics of amorphous pockets created by ion irradiation [28]. In these cases, IV
pairs interact strongly with each other and form more stable structures, responsible for the plateaus in the curves. Recrystallization then requires the collective movement of several atoms which produces a sudden decrease in the potential energy per atom. All these results indicate that amorphization can be achieved without the intervention of any additional defect, and also that amorphous pocket characterization can be studied by IV pair accumulation.

**Figure 5.** Time evolution of the potential energy per atom in lattices with 10, 20, 25 and 30% of IV pairs during annealing at high temperature. Dashed lines indicate the mean potential energy per atom in amorphous and crystal Si, $E_{AM}$ and $E_C$, respectively. Arrows indicate plateaus followed by steep decreases.

To get some insight about the influence of the damage morphology on the recrystallization behavior, we performed MD studies in crystal lattices where we introduced an IV pair concentration of 8%. In one set of simulations IV pairs were distributed randomly in the lattice, separated each other by a distance of at least 4 Å. In other set of simulations IV pairs were arranged in a sphere with a radius of 12 Å [29]. The lattice with scattered IV pairs would represent damage generated by light ion implantation, while the system with concentrated IV pairs would represent damage generated by heavy ion implantation [30]. Both types of systems were annealed at several temperatures, and in all cases the scattered damage disappeared long before the concentrated damage. This indicates that even though the amount of IV pairs was the same, the dynamics of the recrystallization process is totally different. In figure 6 we show the recrystallization velocities for both types of systems as a function of temperature. They have Arrhenius behavior. The activation energy for the scattered damage is very close to that corresponding to isolated IV pair recombination, 0.43 eV. This indicates that a 4 Å separation among IV pairs was long enough to prevent their interaction. In the case of the concentrated damage the activation energy is higher and recrystallization dynamics slower. Recrystallization starts from the amorphous/crystal (a/c) interface, as it is also observed in experiments [31,32]. This is because IV pairs in contact with crystalline atoms are less stable than IV pairs near the center of the sphere. However, their strong interaction with IV pairs in the amorphous side of the interface make them more stable than if they were isolated. This effect is increased in the case of a planar a/c interface, whose recrystallization velocity obtained by MD is also plotted in figure 6.
It shows even higher activation energy for recrystallization, 2.44 eV [29], in very good agreement with the experimental value, 2.7 eV [33]. IV pairs that lie on the planar interface are surrounded by more IV pairs than those on the amorphous sphere. In the limit, as already stated, a pure amorphous matrix would be described by IV pairs completely surrounded by other IV pairs. The recombination of such an IV pair would be equivalent to the generation of a crystal embryo in the amorphous phase. The activation energy for crystal nucleation in amorphous Si has been experimentally determined to be 5 eV [34]. Consequently, the higher the number of surrounding IV pairs, the higher the activation energy for IV pair recombination.

Figure 6. Arrhenius plot of the recrystallization velocity in lattices with scattered and concentrated damage. The recrystallization velocity of a planar a/c interface is also shown. Lines are best fits to each data set. Activation energies are also shown.

MODELING AMORPHIZATION AND RECRYSTALLIZATION

As it has already mentioned, results obtained from these fundamental simulation methods cannot be directly compared with experimental observations. However, based on these results it is possible to develop an atomistic model simple enough to be implemented in a kMC simulator able to reach experimental scales [35]. The IV pair is used as the elementary unit to describe the amorphous material. IV pairs form when Si self-interstitials and vacancies are within the capture radius of each other, and also directly during the collision cascade. Each IV pair is locally characterized by the number of surrounding IV pairs. Its recombination rate decreases as the number of IV neighbors increases. This local description of the disordered zones allows the model to capture any damage morphology that may arise from irradiation cascades, as well as the characteristic regrowth behavior observed in the experiments. The regrowth of amorphous regions starts by IV pairs placed in interfaces with crystalline Si. Each amorphous region regrows at a rate that depends on the local coordination of defects. A continuous amorphous layer is just a particular case of an amorphous pocket. In the planar interface all IV pairs have on average the same number of neighbors. When one of these IV pairs recombines it leaves a “hole”, a small crystalline zone, at the interface. The surrounding IV pairs are left with one less neighbor and therefore they recombine faster. The first IV pair recombination acts thus as a triggering event for the layer-by-layer recrystallization.

This simple model based on the IV pair quantitatively captures the kinetic features related to the ion-induced amorphization and recrystallization in Si, and it is able to give information of
technological relevance. One of the most complex phenomena to reproduce is the critical equilibrium between amorphization and recrystallization depending on dose-rate and temperature [36]. As it can be seen in figure 7, given a dose-rate value there is a critical temperature above which it is not possible to amorphize. Dose-rate specifies the time interval between implant cascades. For low dose-rates, generated damage may anneal out long before the next cascade arrives into the same target region. For high dose-rates, generated damage may overlap with damage created by previous cascades favoring the formation of more stable structures and thus its accumulation. It is important to note that the critical regime between amorphization and recrystallization is determined by a narrow temperature window. If no special care is taken to maintain fixed the wafer temperature during implantation, small variations may lead to very different damage profiles.

![Figure 7](image)

**Figure 7.** Amorphous fraction versus substrate temperature for 1 MeV Si implants to a dose of $10^{15}$ cm$^{-2}$ with several dose-rates (in cm$^{-2}$s$^{-1}$). Solid symbols correspond to the experimental data of Ref. 36, and solid lines represent our simulation results.

![Sub-amorphizing and Amorphizing](image)

**Figure 8.** Snapshots taken during the annealing at 800ºC of a sample implanted with 5 keV $10^{14}$ cm$^{-2}$ Si ions (sub-amorphizing) and 5 keV $10^{15}$ cm$^{-2}$ Si ions (amorphizing). IV pairs are plotted as green circles, whereas Si interstitials and vacancies are indicated by blue and red circles, respectively. Top images show the as-implanted damage profiles.
Whether the implantation is amorphizing or not has important consequences regarding the amount of residual damage left in the lattice. Snapshots shown in figure 8 correspond to the annealing of sub-amorphizing and amorphizing implants. In the former case, the as-implanted profile shows crystalline islands surrounded by large amorphous regions. Upon annealing, amorphous regions recrystallize, releasing to the lattice the unbalanced atoms they contain. These defects accumulate around the mean projected range of the implant, and the amount of retained Si self-interstitials is approximately the implanted dose (+1 model [37]). In the annealing of an amorphizing implant, defects contained in the continuous amorphous layer are swept towards the surface as the a/c interface advances. A band of extended defects is formed only at the end-of-range region, and the amount of stored self-interstitials is significantly lower than the implanted dose.

It is also important to accurately predict the position of the a/c interface in amorphizing conditions, since differences in the amorphous layer depth translate into significant variations in the amount of residual damage. To illustrate this we have plotted in figure 9 the amount of residual damage after solid-phase epitaxial regrowth (SPER) obtained after the implantation of 12 keV Si ions to a dose of \(8 \times 10^{14} \text{ cm}^{-2}\) at a temperature of 20°C, using two different dose-rates. Although the differences in the a/c interface depth are small, of just a few nm, residual damage obtained for the higher dose-rate is approximately 50% of that obtained for the lower dose-rate. Since the implant dose is the same in both cases, profiles of the implanted ion are practically the same. Upon anneal, generated damage recombine and only the excess interstitials generated by the implanted ion survive. When a continuous amorphous layer is formed, the excess atoms contained in the layer are swept towards the surface as regrowth takes place, and only the excess interstitials beyond the initial a/c interface remain. A deeper amorphous layer implies the removal of a larger amount of interstitials, and hence a reduced residual damage. Wafer temperature plays a similar role on the a/c interface depth and the remaining residual damage. If temperature rises during implantation, especially due to the use of high dose-rates, dynamic annealing may lead to an amorphous layer a few nanometers thinner and consequently to a larger amount of residual damage.

![Figure 9](image_url)

**Figure 9.** Simulated damage profile after implant and residual damage after SPER for a 12 keV \(8 \times 10^{14} \text{ cm}^{-2}\) Si implant for two dose-rates: \(2.5 \times 10^{11} \text{ cm}^{-2}\cdot\text{s}^{-1}\) (solid lines) and \(8.3 \times 10^{14} \text{ cm}^{-2}\cdot\text{s}^{-1}\) (broken lines). Profiles of the implanted ion and positions of the a/c interface are also shown.
CONCLUSIONS

In this paper we have shown how atomistic simulation techniques can be used to develop Si-processing models with predictive capabilities. These models have to be physically based and accurate enough to give not only qualitative but also quantitative information. The atomistic simulation techniques have to be organized in a hierarchical scheme in order to be able to reach the size and time scales typical of actual Si processing. To illustrate this simulation scheme, we have presented a fully atomistic model for the ion-beam induced amorphization and recrystallization in Si to be used in front-end processing simulators. It is based on the IV pair as the elementary unit to describe the amorphous phase. According to classical MD simulations, the model considers that the IV pair recrystallization rate depends on the local density of surrounding IV pairs. This simple model is able to reproduce most of the experimental observations. It consistently encompasses ion-induced damage ranging from individual defects to full amorphous layers, and thus amorphization needs not to be specified as an input condition but it is the result of the simulation itself. Consequently, it allows to extend the kMC approach to high implant doses, and therefore the atomistic simulation of the fabrication of nanometer-sized Si devices.

ACKNOWLEDGMENTS

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