Atomistic simulations in Si processing: Bridging the gap between atoms and experiments

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Abstract

With devices shrinking to nanometric scale, process simulation tools have to shift from continuum models to an atomistic description of the material. 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 fed into less detailed simulators which allow direct comparison with experiments. This scheme will be illustrated with the modeling of the amorphization and recrystallization of Si, which has been defined as a key challenge in the last edition of the International Technology Roadmap for Semiconductors. The model is based on the bond defect or IV pair, which is used as the building block of the amorphous phase. The properties of this defect have been studied using ab initio methods and classical molecular dynamics techniques. 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. This approach provides physical insight on the amorphization and recrystallization mechanisms and a tool for the optimization of solid-phase epitaxial-related processes.

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1. Introduction

Silicon processing is facing an increasingly high level of complexity as a result of the current efforts to progress into the deep submicron IC technology. This situation is becoming critical 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 doping techniques into the nanometer regime [1]. Ion implantation is the most prevalent method for adding dopant atoms, since it provides excellent spatial and dose control as well as ease of manufacture. The Si substrate needs to be subsequently annealed in order to electrically activate the dopants and to heal the lattice defects generated during the implantation, which range from point defects and point defect clusters to full amorphous layers depending on implantation conditions. Annealing is done at temperatures high enough to allow the dopant atoms to diffuse to substitutional sites, and for the lattice defects to recombine. This process is highly transient and it is governed by the diffusion and complex interactions between dopant atoms and defects, and especially by the dynamics of clusters of these two.

With further reduction of the devices feature size, new effects or effects that were neglected so far become relevant and compromise the reliability of the manufacturing process. Their experimental characterization is a complex task, firstly because the realization of test lots results extremely expensive, and secondly because these effects usually occur simultaneously which makes the interpretation of measurements very difficult. In this situation the use of predictive process simulation techniques becomes almost imperative. To be predictive, simulators must rely on accurate models which in turn have to be physically based [2].

Most process simulators used in industrial applications are based on continuum methods. In this type of simulators 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]. The reaction rates are defined according to the parameters that characterize their interactions. The numerical solution of these sets of non-
linear partial differential equations requires spatial and temporal discretization to reduce the derivatives into algebraic differences. The problem is converted to a large, nonlinear system of coupled equations, which are solved using standard numerical methods. These 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, which traditionally have been just used to extract continuum model parameters, become a good alternative even for industrial applications [1,5].

In this paper we will 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 our attention in 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 last edition of the International Technology Roadmap for Semiconductors [2].

2. Atomistic simulation techniques

In atomistic simulation techniques the system under study is described taking into account its discrete nature, i.e., as a set of interacting atoms or molecules. Depending on the accuracy used to describe the particle interactions it is possible to distinguish several techniques. In the so-called ab initio methods, the Schrödinger equation is solved for the set of particles (nuclei and electrons) which constitute the system under study. Even though this resolution is carried out using several approximations, this technique provides an accurate description of the interactions based on the electron distribution of the atoms, with no free parameters [6]. However, these methods are computationally very expensive, and thus they can only handle systems of a few hundreds of atoms and are limited to extremely short times. Nevertheless, they are useful to calculate the energies of specific atomic configurations and give excellent insight into the underlying physics [7]. For example, ab initio methods were used to study and provide parameters on the diffusion mechanism of interstitial B in Si [8,9]. Classical molecular dynamics (MD) simulations describe the atomic interactions by empirical force laws which include several parameters [10] chosen by fitting to experimental data or ab initio calculations [11,12]. It is possible to simulate systems containing thousands of atoms for times of the order of nanoseconds, but at the expense of losing the electronic description of the system. MD simulations reproduce the actual dynamics of all system atoms and thus it is possible to determine diffusion paths, evolution among different atomic species must be specified. Unlike MD, the vibrational movement of the Si lattice atoms is not simulated, only the dynamics of the defects and the dopants is followed, which allows the simulation of systems of hundreds of nanometers, i.e., the size of today’s devices. The simulation time-step is variable. It may go from $10^{-7}$ s for some diffusing species, to $10^{-5}$ s, or even longer, for the emission of defects from stable clusters. Generally the fast events tend to disappear quickly leaving slower events that raise the time-step. This allows to easily access to macroscopic times, and so to the simulation of actual processing.
After presenting the main methods of atomistic simulation, it is easy to realize that no individual technique can be used alone for the simulation of actual front-end Si processing. Each one gives information at a different scale level, sometimes complementary, so all of them have to be used in a hierarchical or multi-scale scheme to achieve full processing simulation. 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. 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. The parameters extracted form these detailed atomistic techniques, or even from experimental measurements, along with the mechanisms of defect interactions and diffusion, will define the relevant events to be considered in the kMC simulator (the event catalogue is considered to be complete when able to reproduce the experimental observations). The BCA code is used to generate the implantation cascades. The coordinates of generated defects are fed to the kMC simulator at time intervals determined by the dose-rate. During the inter-cascade time, defect diffusion and interaction events occur at a rate that depends on the sample temperature, thus accounting for the dynamic anneal during the implantation process. This procedure is repeated until the specified dose is reached. Afterward, subsequent anneals can be simulated.

3. Modeling amorphization and subsequent recrystallization

Since the beginning of the use of ion implantation for the fabrication of Si devices, ion-beam-induced amorphization and solid-phase epitaxial growth (SPEG) in Si have been the subject of a great number of studies. There is now a renewed interest in the modeling of these processes because of their technological relevance for the semiconductor industry. For example, high-impedance doses of As or BF₂ are required to achieve high levels of carrier concentration induce amorphization of the Si lattice. In the case of B implantation, preamorphizing Ge implants followed by SPEG are carried out as a way of obtaining high electrical activation with reduced thermal budgets [20].

Traditionally, amorphization was modeled in a very simplistic way. It was assumed that the lattice turned amorphous if a critical point defect concentration was exceeded [21]. Recrystallization occurred instantaneously, resulting in a free-of-defects crystalline zone. Only defects beyond the amorphous-crystal interface remained. One of the main limitations of this simplistic model is the uncertainty in the critical point defect concentration value. Different authors have reported values ranging between \(10^{17}\) and \(10^{20}\) cm\(^{-3}\) depending on the implant parameters (see Ref. [22] and references therein). This uncertainty leads to variations of a few nanometers in the predicted depth of the amorphous-crystal interface and to changes up to 50% in the residual damage concentration beyond it [22]. The exact amount of the residual damage is of great relevance for technological purposes as it significantly affects dopant diffusion and activation. Therefore, it is essential to develop ion-induced amorphization and recrystallization models, compatible with process simulators, which are able to capture the features of the crystal-amorphous transition and its dependence on implant parameters.

To be predictive, an atomistic model for the ion-induced amorphization and subsequent recrystallization of Si must be able to describe, even quantitatively, most of the experimental observations: (a) the annealing behavior of amorphous pockets is not associated to a unique activation energy, rather than a smooth exponential decay plateaus and step regions are observed [23]. (b) Amorphous pockets with similar sizes show a totally different regrowth behavior [23]. (c) Pre-existing amorphous pockets or planar amorphous-crystal interfaces act as nucleation sites in conditions where significant dynamic anneal occurs [24,25] (d) The superlinear dependence of the accumulated damage versus dose [26]. (e) The existence of a critical temperature depending on dose-rate above which it is not possible to amorphize [27,28].

3.1. Fundamental studies

In order to develop models that describe amorphization and recrystallization processes at the atomic level it is essential to identify the defect or defects that can act as amorphous embryos, and those that induce recrystallization. It is generally believed that crystallization [29] and amorphization [30] under irradiation are related to each other and both processes are generally ascribed to ion-beam-induced defects [31]. In the literature, several defects have been proposed to be relevant in the amorphization and/or recrystallization mechanisms: vacancies [32,33] and vacancy complexes [34–36], self-interstitial clusters [37–39], pairs of di-vacancies and di-interstitials [40], dangling bonds in the amorphous phase [41], kinks along [1 1 0] ledges in the amorphous-crystal interface [31,42], and bond defects [43,44]. Among all of them, we have chosen the bond defect to base our atomistic model for amorphization and recrystallization, for the reasons we will expose in the following.

Tang et al. encountered the bond defect when studying self-diffusion and interstitial-vacancy recombination in Si using TB techniques [43]. They found that when a vacancy approaches a (1 1 0) 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. This defect, represented in Fig. 1, consists of a local rearrangement of bonds in the crystal with no excess or deficit of atoms. As 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. Information regarding the structure and energetics of this defect has been extracted using ab initio [45,46], TB [43] and classical MD techniques [47]. The IV pair formation energy, 3.26 eV [45], is of the order of the corresponding to typical point defects in Si. Its equilibrium concentration should then be comparable or even larger than that of the other defects. However, the IV pair has not yet been detected experimentally, maybe because perfect four-fold coordination (which means no unpaired electrons) precludes its detection in standard experiments such as electronic paramagnetic resonance and electron nuclear double resonance. It has
Fig. 1. Atomic structure of the IV pair. 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 IV pair.

also been shown by ab initio techniques that the IV pair hardly disturbs the band structure of Si, which makes it undetectable in the deep level transient spectroscopy technique [46]. Using classical MD techniques, Stock et al. observed that the bond defect can be generated not only by incomplete interstitial-vacancy recombination, but also as a result of a pure ballistic process [44]. 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. They showed as well that the IV pair is a characteristic structural feature of the amorphous-cystal interface [44,48].

As already mentioned, the IV pair is a metastable defect. It spontaneously annihilates by the reverse movement of atoms A and A’ of Fig. 1 toward the perfect lattice positions, switching again their bonds with atoms B and B’. Using classical MD simulations [49], we showed that the IV pair lifetime follows an Arrhenius behavior over a wide temperature range with an activation energy of 0.43 eV [47]. 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 Si lattice. In Fig. 2 we show the temperature evolution at different temperatures 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 lattice, \( E_C \), are also shown. As can be seen, mean potential energies in lattices with starting concentrations of 10 and 20% of IV pairs decreased to the value corresponding to the perfect crystal for all the simulated temperatures. This indicates that fully recrystallization occurred. However, in the case of the sample with 30% of IV pairs the mean potential energy decreases only to the \( E_{AM} \) level, for all the simulated temperatures. Samples with 30% of IV pairs were structurally identical to a pure amorphous matrix, as we determined by calculating the pair distribution function [47]. It is interesting to note that the behavior of the lattice with an initial IV pair concentration of 25% depends on temperature. For \( T=1000 \) K it returns to the perfect crystal, though initially the potential energy per atom is higher than \( E_{AM} \), while it amorphizes for \( T=1600 \) K. After introducing 25% of IV pairs, there are some traces of crystallinity left which act as a seed for crystal recovery at 1000 K, but further thermal agitation at \( T=1600 \) K dissolves these traces and amorphization takes place. Temperature then plays an important role in the amorphization process: higher temperatures favor the recombination of the defects produced during the irradiation, and thus prevent the damage accumulation, but if the defects have accumulated and are interacting strongly, higher temperatures favor
amorphization. On the other hand, for the case of $T = 1200$ K, the potential energy per atom stays between the levels corresponding to amorphous and crystal Si. At this temperature, the system with an IV pair concentration of 25% started to recrystallize, but with a small misorientation with respect to the original perfect lattice due to thermal agitation. In real Si such a situation would correspond to the formation of low-angle grain boundaries, as it has been experimentally observed [50,51].

As can be deduced from Fig. 2, the higher the temperature, the higher the recrystallization velocity for the same concentration of IV pairs. For lattices with a concentration of 10% the energy decay is exponential, which suggests a single activation energy. Effectively, we observed that decay times in these cases followed an Arrhenius behavior with an activation energy of 0.45 eV, very close to the barrier obtained for IV pair recombination. This means that 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 there is just one IV pair. On the other hand, for higher concentrations the evolution of the potential energy per atom shows plateaus followed by steep decreases, indicated by arrows in Fig. 2. This behavior has been also observed in classical MD studies [52] and experiments [23] on the recrystallization kinetics of amorphous pockets created by ion irradiation. In these cases, IV pairs interact strongly with each other and form more stable structures, responsible for the plateaus in the curves of Fig. 2. Recrystallization then requires the collective movement of several atoms which produces a sudden decrease in the potential energy per atom.

The MD simulation results presented so far prove that when IV pairs are present in the Si lattice to a given concentration (around 25%), amorphization of the Si lattice takes place. The resulting structure is identical to the corresponding to a pure amorphous Si matrix. It has been shown by ab initio techniques that low-density extended Si crystals known as "silisil" can be also formed by IV pairs [53]. Consequently, the consideration of the Si amorphous phase as an extended IV network (a microscopic mix of such silisil phases) is physically sensible. On the other hand, the amorphous zones created by IV pair accumulation and those by direct irradiation showed the same features, as far as energy content, internal structure and recrystallization dynamics are concerned. 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. This procedure of accumulating IV pairs can serve then as a controlled way to introduce damage in the silicon lattice.

To get some insight about the influence of the damage morphology on the recrystallization behavior, we have carried out two different classical MD studies [49]. In the first one, we have performed simulations at several temperatures in systems consisting of 2268 atoms where we have 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 0.4 nm. In other set of simulations IV pairs were arranged in a sphere with a radius of 1.2 nm. The lattice with scattered IV pairs would represent damage generated by electron irradiation or light ion implantation, while the system with concentrated IV pairs would represent damage generated by heavy ion implantation [52]. 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 Fig. 3 we show the recrystallization velocities for both types of systems as a function of temperature. As can be seen, they show Arrhenius behavior over a wide temperature range, with corresponding activation energies of 0.44 and 0.89 eV for the scattered and concentrated damage, respectively. The obtained activation energy for the scattered damage is very close to that corresponding to isolated IV pair recombination, 0.43 eV. This indicates that 0.4 nm separation among IV pairs was long enough to prevent their interaction. In the case of the concentrated damage the activation energy is higher, and thus the recrystallization dynamics slower. Recrystallization starts from the amorphous-crystal interface, as it is also observed in experiments [54,55]. 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 cooperative effect is increased in the case of a planar amorphous-crystal interface, whose recrystallization velocity obtained by MD [49] is also represented in Fig. 3. It shows even higher activation energy for recrystallization, 2.44 eV, in very good agreement with the value measured in the experiments, 2.7 eV [56]. IV pairs that lie on the planar interface are surrounded by more IV pairs than those on the amorphous sphere. In the limit, as we have shown, a pure amorphous matrix would be described by an IV pair completely surrounded by other IV pairs. The recombination of such an IV pair, equivalent to the generation of a crystal embryo in the amorphous phase, cannot be studied by MD techniques because it would imply prohibitively long simulation times. However, the activation energy for crystal nucleation in amorphous Si has been experimentally determined to be 5 eV [57]. Consequently, the higher the number of surrounding IV pairs...
pairs, the higher the activation energy for IV pair recombina-
tion. These energies range from 0.43 eV for an isolated IV pair
to 5 eV for a fully coordinated IV pair.

In a second classical MD study we have used two crystal
lattices consisting of 6084 atoms where we introduced 510 IV
pairs. In one of the simulation systems IV pairs were arranged in
a sphere in the center of the lattice (diameter of 3.4 nm), and in
the other with the shape of a cube (side of 2.7 nm). In this way it
is possible to make a comparative study of the recrystallization
behavior of compact structures of the same size, differenced
only by the arrangement of the crystal–amorphous interface.
Fig. 4 shows several snapshots taken during the annealing of
the two systems at 1400 K. Again, recrystallization starts from
the crystal–amorphous interface. After 240 ps of annealing, ver-
tices and edges of the cube have disappeared, so the damage
structure has become a sphere. Its size is smaller than the sphere
annealed for the same time. After 550 ps, the amorphous cube
has completely annealed out, while some damage still remains
in the case of the sphere. To fully disappear, this damage had
to be annealed for 550 ps more. This behavior can be explained
taking into account the previously commented MD results. The
vertices of the cube are first to recombine since corresponding
IV pairs are surrounded by less neighboring IV pairs and thus
are less stable. Then, next to recombine are IV pairs lying on
the edges of the cube. After this initial process, the cube has
become a sphere with a smaller size that the original sphere
annealed for the same time. This is because IV pairs lying on
the amorphous sphere surface have on average the same num-
er of neighboring IV pairs, a number that is higher than in the
case of the cube vertices and edges, which means that they are
more stable for the same annealing conditions. After 240 ps of
annealing we have two spheres of different sizes. The first to
anneal out and disappear is the smallest one, which corresponds
to the initial cube, since its surface has a smaller curvature radius
and consequently IV pairs lying on it have less IV neighbors.
These results confirm again that recrystallization of amorphous
pockets depends on the amorphous–crystal interface morphol-
ogy, not on pocket size, and they help to explain the experimental
observation where amorphous pockets of apparently the same
size have very different annealing behaviors [23].

3.2. Reaching macroscopic scales: comparison with
experiments

As already mentioned, the results obtained from classical MD
and more fundamental methods cannot be directly compared
with experimental observations, since simulated temperatures
are too high, system sizes too small and simulation times too

![Fig. 4. Snapshots taken during the annealing at 1400 K of two amorphous pockets of the same size (510 IV pairs), but with different geometries: a cube and a sphere. Their size is typical of actual amorphous pockets created by 200 keV Xe irradiation of Si [23]. Colors indicate potential energy (blue: lower energies; red: higher energies).](image-url)
short. However, based on these simulation results we have developed an atomistic model simple enough to be implemented in a kMC simulator and thus reaching experimental scales. BCA provides the initial profile of damage as it results from the dopant implantation in the form of Si self-interstitials, vacancies and IV pairs. These simple defects can agglomerate and form more complex structures leading to defect clusters and amorphous pockets [58]. IV pairs form when Si self-interstitials and vacancies are within the capture radius of each other [43], and also directly during the collision cascade [44]. The IV pair is used as the elementary unit to describe the amorphous material. Each IV pair is locally characterized by the number of neighboring IV pairs. Its recombination rate decreases as the number of neighboring IV pair increases. We assign an activation energy of 0.43 eV to the isolated IV pair (0 neighbors). The experimentally measured activation energy for recrystallization of a planar amorphous–crystal interface, 2.7 eV [56], provides us with another parameter to characterize the recombination rate of IV pairs with about half of the total coordination number. IV pairs embedded into an amorphous matrix (completely surrounded by neighboring IV pairs, and thus with full coordination) have an activation energy of 5 eV [57]. Intermediate coordination numbers have interpolated activation energies [58].

The local characterization of the disordered atoms 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. In the model, the continuous amorphous layer is just a particular case of an amorphous pocket. This naturally accounts for similar regrowth properties of amorphous pockets and continuous amorphous layers observed experimentally [55]. The regrowth of amorphous regions starts by the IV pairs placed in interfaces with crystalline Si because they have smaller number of IV neighbors than the inner defects. Each amorphous region regrows at a rate that depends on the local coordination of defects. Finite-size amorphous pockets (convex in several sides) naturally regrow at lower temperatures because IV pairs at the interface have fewer neighbors than they would have in a planar interface. Differences in the annealing times observed for similar amorphous pocket sizes [23] are captured by the variations in recombination rates (determined by the local IV pair coordination) within different geometries. The step-like behavior of the amorphous pocket recrystallization (see Fig. 2) is easily explained within this model. Plateaus correspond to pockets in which IV pairs lying on the amorphous–crystal interface have the same coordination. The pockets remain stable until one of these IV pairs recombines, leaving a “hole” (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 recombination of the surrounding IV pairs, producing the steep decreases in the pocket sizes. The regrowth of the planar amorphous–crystal interface takes place in a similar fashion: a layer-by-layer regrowth occurs activated by the recombination of the first IV pair in each layer.

This simple model based on the IV pair quantitatively captures the kinetic features related to the ion-induced amorphization in Si. It encompasses and unifies homogeneous and heterogeneous mechanisms. The nucleation of the amorphous phase consists in the formation of IV pair structures with enough number of IV neighbors to be stable. At the appropriate temperatures, these amorphous embryos can be either small IV pair complexes generated in dilute cascades (homogeneous nucleation) or dense IV pair agglomerates formed in the cascades of heavy ions (heterogeneous amorphization). When there is significant dynamic anneal, pre-existing amorphous pockets or planar amorphous–crystal interfaces can act as nucleation sites [24,25]. Isolated IV pairs may not be able to survive by themselves but if they interact with a pre-existing amorphous region, the generated IV pairs will have more IV neighbors and become stable. IV pairs are thus added to the amorphous zone producing its growth.

The cooperative nature of the amorphization phenomena, which is manifested in the superlinear behavior of the accumulated damage versus dose, is a consequence of the increased stability of the IV pairs with the number of IV neighbors. Fig. 5 shows the experimental [26] and simulated results on this matter for a 100 keV Si implant at room temperature. For low doses the amorphous fraction grows slowly until a sharp increase occurs near a given (transition) dose. This happens because the damage is dilute for low doses, so only a small percentage of the generated damage survives (region I). As the dose increases and the damage reaches certain level, IV pairs start interacting and become more stable. Therefore, a larger percentage of the generated damage survives, resulting in its superlinear increase with dose (region II). The process of adding more damage saturates when amorphization is reached and new cascades just move atoms already displaced from their lattice positions (region III).

One of the most complex phenomena to model is the critical equilibrium that occurs between amorphization and recrystallization processes in Si as the lattice tends to recover from damage generated during ion-beam irradiation. The implant dose-rate (time between successive cascades) and substrate temperature determine the probability of the damage from each cascade surviving until the arrival of a new cascade, and thus the rate of damage accumulation. The effect of the dose-rate
and temperature for 1 MeV Si implants is represented in Fig. 6. As can be seen, the critical temperature for amorphization, $T_c$, lies around room temperature [27]. The amorphous fraction (IV pair concentration relative to the atomic Si density) can be parametrized with a simple reverse exponential:

$$\text{amorphous fraction} = a + \frac{b}{1 + \exp[(T - T_c)/c]}$$

where $c$ describes the width of the phase transition, and $a$ and $a + b$ set the limits for $T > T_c$ and $T < T_c$, respectively. In Fig. 7 the critical temperatures for amorphization versus ion flux for Si and Ge implants resulting from our simulations are plotted and compared with experiments [28]. The average lifetime of a given IV pair in an amorphous zone is given by

$$t_b = \frac{E_a}{k_B T}$$

where $t_b$ is the prefactor, $E_a$, the activation energy for recombination, $k_B$, the Boltzmann constant, and $T$ is the temperature. The critical temperature for a given dose-rate corresponds to that at which $t_s \sim t_b$, being $t_s$ the time for arrival of two successive ions to the same region. Because of the exponential temperature dependence, small changes in $T$ induce large variations in $t_s$ and, therefore, in the probability of the defect surviving during $t_s$. An increase in the dose-rate (reduction in $t_s$) shifts the temperature at which $t_s \sim t_b$ toward higher values.

Implantation cascades produce a great variety of damage configurations, and basically the whole spectrum of activation energies from 0.4 to 5 eV are present. For the damage to accumulate and produce a continuous amorphous layer, a fraction of the generated damage in each cascade has to survive. At low $T$ most defects follow $E_a \gg k_B T \ln(t_s/t_b)$ and survive. At high $T$, all defects recombine. In those extreme cases there is no temperature dependence. However, in the regime where damage generation closely balances damage annihilation, several activation energies were measured for the onset of amorphization for different ions [28], which in principle were associated to different defects. In our model, the structural defect that causes amorphization is the same for all ions, but it has different energy barriers for recombination as a function of the surrounding neighborhood. Light ions produce mostly isolated or small IV pair complexes. Therefore, small values of $E_a$ are governing the critical equilibrium that allows the onset of amorphization. On the contrary, heavier ions produce a larger fraction of denser damage structures with larger $E_a$ values. This also explains why the critical temperature for amorphization $T_c$ is higher for heavier ions.

4. 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 captures most of the experimental observations: the superlinear dependence of damage accumulation with dose, the critical regime for the crystal–amorphous transition determined by the dose-rate and implantation temperature, the recrystallization behavior of amorphous pockets and its dependence on amorphous–crystal interface morphology, etc. 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.
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