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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 feed 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.

Keywords: Atomistic simulation; Amorphization; Recrystallization; Ion implantation; Silicon

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-

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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 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 defect configurations [13], and even the damage caused by an energetic ion colliding with a Si lattice [14]. However, it is not feasible to simulate the complete implantation and subsequent anneals, as these processes involve times on the order of seconds or even minutes. The *tight-binding* (*TB*) *technique*, based on the method of linear combination of atomic orbitals [15], aroused as a trade-off alternative between ab initio and classical MD simulations. It is a non-parameter-free approximation [10] that allows the use of system sizes and simulation times intermediate to the ones typical of the previously described techniques while keeping the electronic description of the system. TB simulations have been used, for example, to study formation energies and equilibrium configurations of self-interstitial extended defects in Si [16].

Simulation methods considered so far allow a full description of the system dynamics at the atomic level. However, the time and size scales accessible to them are still orders of magnitude far from experimental conditions. Usually simulations are carried out at high temperatures in order to accelerate system dynamics, and boundary conditions are introduced to minimize finite-size effects. These considerations introduce the first difficulty in trying to relate simulation results with experimental observations: there is no warranty that the system will behave the same way at low temperatures, and also that boundary conditions do not introduce artifacts in the simulation. Another big difficulty arises when analyzing the data obtained from the simulation. Even for a small number of atoms simulated for a relatively short time, the amount of data generated by the simulation (atom positions, velocities, kinetic and potential energies, etc., on each time-step) can be so overwhelming that the task of extracting meaningful information becomes really hard [17].

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 sizes and times 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 ions or Si recoils and the Si target atoms by assuming that the energetic atom interacts only with the closest atom in its neighborhood [18]. This method provides the atomic coordinates of the implanted ion and the generated Si interstitials and vacancies during the collision cascade. Thousands of cascades can be easily calculated to give enough statistical resolution and generate reliable dopant and damage profiles. Ideally, a reduced number of parameters should be enough to describe the nuclear and electronic interactions in the collision of any ion–target atom combination [19]. On the other hand, *kinetic Monte Carlo* (*kMC*) *codes* allow the simulation of the annealing step by only handling dopant atoms and lattice defects and their interactions [1,5]. Parameters that define these interactions, such as binding energies, capture radius, etc., and the diffusion behavior of every 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^{-9} s for some diffusing species, to 10^{-3} 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.