Materials Science in Semiconductor Processing xx (xxxx) xxxx–xxxx

Contents lists available at ScienceDirect

Materials Science in Semiconductor Processing

journal homepage: www.elsevier.com/locate/mssp

Improved physical models for advanced silicon device processing

Lourdes Pelaz*, Luis A. Marqués, María Aboy, Pedro López, Iván Santos

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

ARTICLE INFO

Keywords:
Silicon
Ion implantation
Annealing
Atomistic simulation

ABSTRACT

We review atomistic modeling approaches for issues related to ion implantation and annealing in advanced device processing. We describe how models have been upgraded to capture physical mechanisms in more detail as a response to the accuracy demanded in modern process and device modeling. Implantation and damage models based on the binary collision approximation have been improved to describe the direct formation of amorphous pockets for heavy or molecular ions. The use of amorphizing implants followed by solid phase epitaxial regrowth has motivated the development of detailed models that account for amorphization and recrystallization, considering the influence of crystal orientation and stress conditions. We apply simulations to describe the role of implant parameters to minimize residual damage, and we address doping issues that arise in non-planar structures such as FinFETs.

1. Introduction

The continuous scaling down of electronic devices has revealed the necessity of innovative nanostructures to overtake the limitations of traditional planar MOSFETs in present and future technological nodes [1]. Thus, a change from the traditional 2D planar FETs to 3D multigate MOS devices has been imposed to improve device performance [2–5]. FinFETs [6–8] are already in production at industrial level, while the use of gate-all-around devices [9–11] and nanowire FETs [12–15] is being considered for near-future technology nodes as a promising scaling approach.

Ion implantation is still the most common technique used to selectively introduce dopants in planar and multigate FET devices for junction formation. This technology is also being used for pocket formation, threshold-voltage or work-function adjustment in advanced memory and CMOS devices [16]. Power devices, CMOS image sensors and even solar cells [17] also take advantage of the precise control in the dopant distribution provided by ion implantation. However, as the energetic incoming ions penetrate into the substrate, the crystal lattice becomes damaged. Subsequent thermal anneals are required to heal the crystal defects and to electrically activate dopants. The compromise to remove damage and to control dopant activation and diffusion has driven sophisticated implantation and annealing schemes. Modern devices involve a mixture of implant species, cold and hot implants followed by processing steps at low temperatures (< 650 °C) combined with high temperature anneals with rapid temperature-time variations (flash and laser anneals) [18,19].

Semiconductor technology faces up to continuous challenges to satisfy the requirements of scalability of new devices and low power/high performance. The minimization of defects is a pressing concern in all devices because they are responsible for increased leakage currents, carrier mobility degradation and enhanced dopant diffusivity, among other deleterious effects [20–22]. Variability is also crucial in modern devices compared to past technologies. It is associated to inaccuracy in angle, energy, dose or temperature control during implants, wafer temperature variations, random dopant fluctuations or inhomogeneous defect distributions. In addition, reduced sizes and complex geometries of nanoscale devices introduce additional complexity in the characterization techniques [23].

The fabrication and design of new integrated circuits makes the use of technology computer-aided design tools essential to reduce the development times and costs [24]. In fact, trends in device technology drive the requirements for process modeling. Simulation capabilities evolve to encompass processes, geometries and materials considered for present and future devices. Scaling of transistors does not only demand a higher degree of accuracy but also may require new models for effects that were neglected in previous technology nodes. As the classical Si scaling is reaching its limits and many options are being explored (tunneling devices, quantum electronics, etc. [25]), physics based models should provide understanding and predictive capabilities that could guide technology.

The mainstream tool at industrial level for the simulation and modeling of ion implantation and annealing processes in Si relies on semi-empirical analytical expressions for implanted dopant and defect profiles, and on continuum models in which interactions among dopants and defects are formulated as a series of coupled partial

* Corresponding author.
E-mail address: lourdes@ele.uva.es (L. Pelaz).

http://dx.doi.org/10.1016/j.mssp.2016.11.007
Received 29 July 2016; Received in revised form 20 October 2016; Accepted 3 November 2016
Available online xxxx
1369-8001/

differential equations [24,26]. For enough accuracy and predictability, many interactions should be considered which involve numerous rate equations and unknown parameters. In addition, the presence of very large concentration gradients, high extrinsic doping levels, dopant clustering, dopant segregation, impurities such as C, F or N, amorphous-crystalline (a/c) phase transitions, heavily strained Si and SiGe, and 3D device geometries make this approach difficult and not very efficient.

In this scenario atomistic modeling is gaining relevance in process simulation. Atomistic methods are time consuming as they consider interactions at atomic level, however they are more flexible when applied to systems that require a detailed description or involve complex materials and device architectures. The advances in the understanding of the physics behind dopant-defect interactions and the explosion of computer resources (large memory cells and multiprocessor computers) at an affordable price have greatly contributed to the progress in atomistic process simulation. The reduction of device size and the increase of computer power have enabled full atomistic simulation of real structures. Kinetic Monte Carlo (KMC) models [27,28] are beginning to play an important role, both for fundamental research and as a pathway to improve continuum models, and also for direct process simulation at industrial level [24]. KMC methods are based on the random selection of events and particles (dopants and defects) which are relevant for the particular material and process to be simulated. The probability of occurrence of every event is determined by an activation energy and a pre-exponential factor. Once all events have been assigned a probability, a random number determines which particular event will take place and which particle will be involved. Then, the simulation time is increased accordingly to the selected event frequency. KMC models make use of a large number of parameters which are usually extracted from experiments or more fundamental simulation techniques, such as classical molecular dynamics (CMD) [29,30] or ab-initio methods [31,32].

The prominence of Si in electronic circuits has driven intense research on this material over the past decades, leading to modeling capabilities with a high sophistication level. Nevertheless, existing understanding is still improving, some issues remain unsolved and new challenges are appearing. For instance, just recently unexpected {001} dislocation loops have been observed in laser annealed implanted Si [33]. Defect growth models based on coalescence instead of conventional Ostwald ripening have been proposed to account for such defects [30]. Other materials that are only recently being considered for integration into mainstream devices, such as Ge and compound semiconductors (III-V´s, SiC), have not been researched as much as Si, and there is a lack of understanding even of fundamental parameters and processes [34]. In principle, research on new materials can be built on the experiences and methods developed for Si. But even for Ge, so similar to Si in many aspects, the extrapolation of Si models is not straightforward [35].

In this paper we review atomistic process modeling approaches for issues related to ion implantation in novel devices. We go into detail about the evolution of implantation and damage models, from approximate empirical descriptions to detailed atomistic models, in response to the accuracy demanded in modern process technology. We apply atomistic simulations to describe the role of implant parameters to minimize residual damage and we address doping issues that arise in non-planar structures.

2. Towards a comprehensive description of ion-implanted damage

Ion implantation has been used in Si technology in a routine way. For many years, analytic distributions were used to obtain fast estimations of dopant and damage depth profiles [36]. These profiles were characterized in terms of the projected range and straggling of implanted ions and generated damage. The parameters that define these distributions need to be calibrated for each set of implantation conditions (ion type, energy, incident angle, etc.) Thus, they cannot be used to predict dopant profiles for implantations that have not being previously tabulated. In addition, they do not provide any information at the atomic level of the damage generated during the implantation process. This information is essential to account for dynamic annealing or local inhomogeneities.

Monte Carlo methods based on the binary collision approximation (BCA) overcome this limitation as they provide an atomistic description of individual collision cascades during the implantation process. The basic idea of BCA is that energetic moving ions that penetrate the implanted target only collide with their closest target atom. These collisions can be numerically solved from the energy and momentum conservation laws [37–39]. The target atoms are placed in crystalline lattice sites (such as in MARLOWE [37,40,41] and IIS [42] codes) or in random positions to reproduce an amorphous material (such as in SRIM code [43]). This has consequences in the channeling of the implanted ions and therefore in the tails of the profiles. In any case, a target atom is displaced from its lattice position when its energy after the collision exceeds the displacement energy threshold, E_d [37]. For Si, experimental and theoretical estimations for E_d range from 10 to 30 eV [44–46], but for most BCA simulators it is conventionally taken as 15 eV [40,43]. For energy transfers above E_d, the target atom initiates a recoil, which leaves a vacancy where the collision occurs and generates a Si self-interstitial where the target atom stops. For energy transfers below E_d the target atom is not displaced and the energy is assumed to be lost to phonons [43]. This treatment of implantation cascades allows simulating almost any implantation condition without additional calibrations.

Some BCA simulators only track the trajectory of the implanted ion, and the number of displaced atoms N_{DA} is estimated taking into account the energy deposited into a given target volume E_{dep} using the modified Kinchin-Pease formula [47]:

$$N_{DA}=0.42\frac{E_{dep}}{E_d} \quad (1)$$

Within this approach [48], ion profiles are rapidly evaluated and generally agree with experiments. The depth distribution of dopants and defects is obtained by simulating a large number of implant cascades, but at the expense of losing the atomic description of damage.

To obtain the complete description of the damage generated within BCA, it is necessary to follow the trajectories of the implanted ion and all the generated recoils (*full cascade* BCA). The result of this type of simulation is the position of the implanted ion and the generated Si self-interstitials and vacancies, called Frenkel pairs (FPs), which can be the input for KMC codes. This approach adequately reproduces the dilute damage generated by light ions. However, it is not able to reproduce more complex damage and amorphous structures observed experimentally for heavy ions or molecular implants. These implant conditions have to be properly modeled since ions such as Ge or As are frequently used in the manufacturing of Si devices as preamorphizing steps [49,50], and molecular implants with octadecaborane are considered as an alternative to monatomic B implants because they are self-amorphizing and minimize residual damage [51].

In order to obtain a detailed and accurate description of damage structures generated during cascades it is necessary to resort to CMD simulations. In CMD the interactions among atoms are described through an empirical potential, which is an analytic function developed and fitted to reproduce the equilibrium properties of the simulated material (crystal structure, lattice constant, bulk modulus, melting temperature, etc.) [52]. To correctly account for the high energy collisions that take place during implantation cascades, splines of empirical potentials to repulsive pair potentials are used [53]. Within CMD simulations the dynamics of atoms is obtained by the numerical integration of Newton's equations. These simulations showed that light ions generate dilute damage in the form of isolated FPs or small defect