Materials Science and Engineering B 124–125 (2005) 409–414

www.elsevier.com/locate/mseb

A comprehensive solution for simulating ultra-shallow junctions: From high dose/low energy implant to diffusion annealing

F. Boucard [a,*], F. Roger [a], I. Chakarov [a], V. Zhuk [a], M. Temkin [a], X. Montagner [a], E. Guichard [a], D. Mathiot [b]

[a] *Silvaco Data Systems, 55 Rue Blaise Pascal, F38330 Montbonnot, France*
[b] *InESS (CNRS and Université Louis Pasteur), 23 Rue du Loess, F67037 Strasbourg, France*

Abstract

This paper presents a global approach permitting accurate simulation of the process of ultra-shallow junctions. Physically based models of dopant implantation (BCA) and diffusion (including point and extended defects coupling) are integrated within a unique simulation tool. A useful set of the relevant parameters has been obtained through an original calibration methodology. It is shown that this approach provides an efficient tool for process modelling.

Keywords: Silicon; Dopant; Diffusion; Implantation; TCAD; Process modeling

1. Introduction

The persistent semiconductor technology trend of shrinking down device size requires development of very aggressive technological setups consisting in high dose/low energy implants, followed by rapid thermal anneals (RTA). Since it is now well established that phenomena involved in ion implantation will play a key role in transient enhanced diffusion (TED), advanced process simulation tools need to model accurately these two steps for deep submicron CMOS technologies. This paper presents the comprehensive solution fully integrated into the commercial SILVACO TCAD suite needed by advanced process technology designers. The implantation step simulated with a Monte-Carlo code based on the binary collision approximation (BCA), provides initial impurity and defects profiles. The diffusion simulation includes the latest physical model developments: dopant–defect pair, interstitials or vacancy clusters and mixed dopant–defect clusters formation and evolution. Although the complete model covers a wide range of physical interactions, it is straightforwardly usable thanks to a comprehensive set of parameters obtained using an original calibration methodology and a dedicated partial differential equation solver to optimize simulation time.

* Corresponding author.
E-mail addresses: Frederic.Boucard@silvaco.com (F. Boucard), Daniel.Mathiot@iness.c-strasbourg.fr (D. Mathiot).

0921-5107/$ – see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.mseb.2005.08.120

2. Implant and diffusion models

Ion implantation and radiation damage are modelled by means of a simulation technique based on the '*BCA*'. The principal assumption of this approximation is that the interaction of energetic particles may be separated into a series of two-body encounters. The real benefit of this approach is the moderate speed of calculation combined with the possibility of including single-crystal structures in the calculation. The slowing down of energetic particles is a result of nuclear and electronic stopping. An universal Ziegler–Biersack–Littmark (ZBL) screening function is used for the interatomic potentials, while the electron stopping is modelled through *local* and *non-local* contributions to the inelastic energy losses. The *non-local* is that of Wang et al. [1], and the local stopping is calculated using the technique of Azziz et al. [2], with a correction for high energies when energy transfer diminishes as described in Ref. [3].

In order to simulate the radiation-induced damage, the model accounts for all collision events within the collision cascade. As demonstrated elsewhere [4], up to 80% of the created *I–V* pairs can annihilate due to recombination, so, the local arrangement of the displaced atoms and vacancies, from where these atoms originated, becomes important when spontaneous recombination has to be taken into consideration. Furthermore, it is not only the number of defects but also their initial spatial distribution, which influences the residual damage. This pertains, especially to rearrangement of defects (formation of clusters, loops, voids,

etc.) before subsequent migration and thermal annealing is precluded. As a first approach to the initial distribution of defects, at the completion of the cascade, the model of Snyder and Neufeld [5] is used. The value of the vacancy capture radius was carefully chosen so that the amount of residual damage is comparable to that calculated with other techniques, e.g. kinetic Monte-Carlo.

The full advanced diffusion model will use as initial input, the impurity and defects profiles calculated previously with the BCA code. This model is made of three separated parts, each one corresponding to one particular phenomenon, dynamically interacting with each other [6].

The classical dopant diffusion model [7] takes into account all the known couplings existing between the dopant and point defects (self interstitials and vacancies). All the charge states experimentally established for both the point defects and dopant–defects pairs are considered. The local equilibrium is not assumed for the various formation/dissociation reactions, thus the full system of continuity equations for both dopant, point defect and clusters is dynamically solved. Moreover, a model has been implemented for dopant precipitation when the solid solubility limit is reached.

The second component of the model deals with defect clustering effects, where some of residual excess point defects nucleate and evolve into various forms of interstitial clusters (IC) like $\{3\,1\,1\}$ defects, dislocation loops or vacancy clusters (VC). This evolution is explained by a competitive growth and dissolution of interstitial or vacancy clusters. These phenomena are described by the Ostwald ripening theory based on the reduction of free energy per defect of the extended defect, which leads to the growth in size of the clusters during annealing [8,9]. This phenomenon drives the point defect super saturation and therefore modifies the dopant diffusion and clustering behavior.

Eventually, another part of excess point defects will trapped dopant atoms, to form immobile complexes, which makes up the third part of the model. In case of boron implantation, the model takes into account the formation of boron interstitial clusters (BIC), like BI_2^+, B_2I^0, $B_3I_2^+$, $B_4I_3^+$, where charge states are also considered according to Ref. [10]. While in the case of arsenic implantation, As atoms aggregate preferentially with vacancies to form As_2V^0 or As_4V^0 complexes. This clustering phenomenon leads to an unwanted inactivation and immobilization of the implanted species.

Moreover, this simulation tool is flexible and expandable since other phenomena which may affect the dopant diffusion, i.e. the presence of carbon or fluorine atoms, can be easily incorporated by simply adding new chemical reaction and its coefficients to the model file. The use of such a complex physically based model involves many parameters, which can be accurately determined only by a calibration methodology presented hereafter.

3. Calibration methodology

The diffusion model presented above has up to 40 physical parameters including formation energies, kinetic coefficients, etc. Having in mind to keep them physically significant, an original calibration methodology has been developed [11]. It is based on specific statistical strategies, which include screening and sorting of relevant parameters, design of experiments (DoE) and responses surface models (RSM) optimizations. This has been applied sequentially to all three components of the diffusion model. This calibration methodology has been successfully used on a broad range of experiments. Relevant simulations are presented below.

4. Simulation results

A complete set of simulations has been performed using both BCA implant and advanced diffusion models. First, the interstitial clusters part of the model has been validated using the experimental data obtained by Cowern et al. [12] (Figs. 1 and 2). Briefly, this experiment consists in observing the diffusivity of two boron marker layers after a silicon implantation at 40 keV to a dose of 2×10^{13} cm^{-2}. As exhibited in Fig. 2, the model accurately predicts the two stages of the diffusion acceleration: the first plateau appearing at the earliest stage of the annealing, governed by the formation of small interstitial clusters, the second one characteristic of the competitive growth of $\{3\,1\,1\}$ defects. Secondly, the calibration procedure was applied to tuning of the Pelaz experiment [13] in which a buried boron layer with a peak concentration above the 10^{19} cm^{-3} level is annealed at 800 °C for 35 min in the presence of defects created by a 2×10^{13} cm^{-2} silicon implant. It can be seen in Fig. 3 that substantial portion of boron concentration may be kept immobile and inactive even below the solid solubility level, because boron atoms are trapped in mixed clusters (boron interstitial clusters). The two previous experiments were used to calibrate the diffusion model.

As a validation test of the ability of our diffusion model to handle all the interactions existing during the dopant diffusion, three most representative implantation/diffusion experiments were chosen for simulations. The first experiment presented in

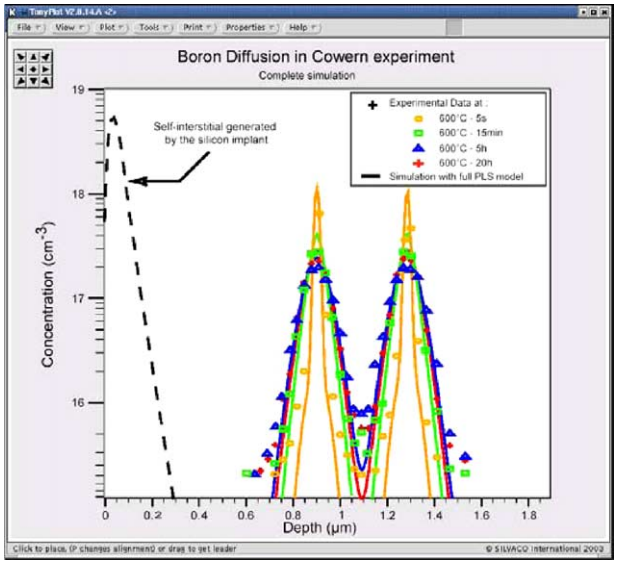

Fig. 1. Simulation (solid line) of Cowern experiment (symbols) [12], where two boron MBE-pics diffuse after a Si implantation at 40 keV/2×10^{13} cm^{-3}. During the annealing, interstitial clusters will evaluate following through an Ostwald ripening scheme and will control the acceleration of the dopant diffusion.