

Simulation Standard

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CNET Physical Diffusion Model Included in ATHENA

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INTRODUCTION

With the growing complexity of integrated circuit manufacturing technology, process and device simulators have become nowadays essential tools for the design of small geometry devices. The ultimate goal of an ideal simulator is to compute the electrical characteristics of a given device, by using only process-related data as input parameters. Since the device electrical characteristics depend drastically on the distribution of the electrically active impurity (dopants), resulting from the entire thermal processing sequence, it is of prime importance for the process simulator to use diffusion models as accurate as possible. This is particularly important for deep sub-micron processes. Indeed, for these emerging technologies, 2-D or even 3-D phenomena are expected to be of growing importance, whereas there is at the present time no accurate technique to measure multi-dimensional dopant profiles. As a consequence, the active dopant 2-D distributions can only be obtained by simulations, which have to be based on models as reliable as possible. In the last decade, it has become clear that the various "abnormal" behaviors of dopant diffusion in Si are caused by the existence of non-equilibrium point defects, either induced by the diffusion process itself (emitter push effect caused by high concentration P diffusion), or injected into the substrate by external treatments, such as oxidation or nitridation, or resulting from the ion implantation used to introduce the dopants into the Si substrate. With the necessary decrease of the thermal budget linked to the shrinkage of the device dimension, these transient phenomena become key points for accurate dopant diffusion simulation. About one year ago (January 1995) SILVACO and CNET-Grenoble (France Telecom) signed a cooperation agreement, the purpose of which was to implement into ATHENA the dopant diffusion model developed at CNET. In this article we briefly describe this model, emphasizing on the differences with the standard full.cpl model of ATHENA, and we present some typical simulations obtained with a Beta version of ATHENA (3.1.8.B) including this model.

MODEL DESCRIPTION

The basic formalism to describe the coupled dopant/point defects system has been laid out at CNET by D. Mathiot and J.C. Pfister(1). This formalism is also the base of the standard full.cpl model of ATHENA, and thus the complete CNET model is actually an extension of the full.cpl model, allowing a better description of the diffusion phenomena particularly at very high dopant concentration.

We describe below the main physical points taken into account in the model, evidencing when necessary the special features of the CNET model:

- i) Dopant diffusion of all the dopants is assisted by both the vacancies (V) and the self-interstitials (I). These point defects exist in various charge states, the relative concentrations of which depend on the local Fermi level position, i.e. on the local dopant concentration.
- ii) Both I and V have strong binding energies with the dopant atoms, and as a consequence the diffusing species are dopant/defect pairs (the isolated substitutional dopants are immobile). These impurity/defect pairs, in their various charge states, are assumed to be in local equilibrium with the free substitutional dopant atoms and the free defects. In the CNET model, at high dopant concentrations, the concentrations of these pairs are not considered as negligible with respect to the substitutional (active) dopant concentration. In consequence, their concentrations are explicitly taken into account to compute the total dopant

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concentration and the Fermi level position (i.e. carrier concentration). A direct consequence is a partial self-compensation at high doping concentration, contributing to the differences between total and active concentrations, and affecting the variations of the extrinsic diffusivities as a function of the total doping.

- iii) In the case of As and B at concentrations approaching the solid solubility limit, neutral and immobile complexes (As_2V or B_2I) are formed, which decrease the effective diffusivity and contributes to the inactive dopant concentration. At the present time, these complexes are assumed to be in local equilibrium with the other species. An extension of the model accounting for a dynamic clustering(3) is foreseen.
- iv) When the dopant concentration exceeds a few 10^{20} cm^{-3} , the dopant/V pairs can no longer be considered as isolated entities, because the vacancies can interact with more than one dopant atom. In CNET model this is described by the existence of a "percolation" cluster of dopant atoms in fifth neighbor position from each other(2). In this cluster both the effective diffusivity and concentration of the vacancies are strongly increased, causing a strong enhancement of the vacancy-assisted diffusion component. This mechanism permits an accurate description of the famous "kink and tail" shape of the high concentration predeposition profiles for phosphorus.
- v) The flux of each diffusing species (dopant/defect pairs and free defects) include drift terms caused by the built-in electric field due to the dopant gradients.
- vi) (I) and (V) are not considered at local equilibrium, but they can annihilate by bimolecular recombination. A specific feature of CNET model is that these annihilations take place not only between the free defects, but also involve the impurity defects pairs, which play the role of recombination centres. As a consequence the I-V recombination rate is strongly enhanced at high dopant concentration.

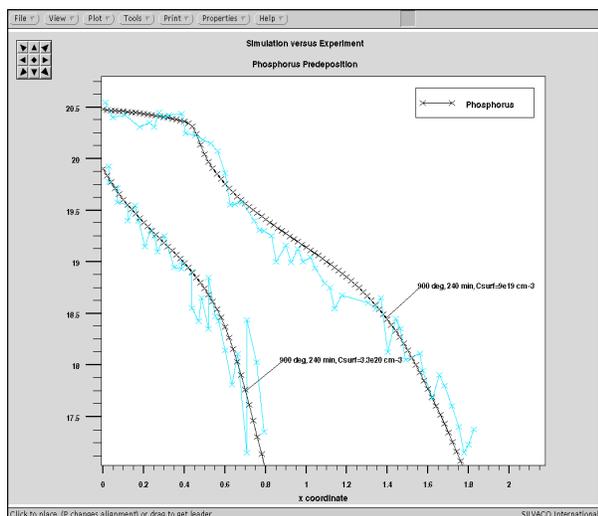


Figure 1. Comparison between experimental and simulated profiles at 900°C. The experimental results are from Refs.[4,5], and the simulations are performed with the CNET model.

EXAMPLES

To illustrate the improvements given by the CNET model, we show simulations of phosphorus predeposition profiles at high and intermediate surface concentrations. Figures 1 to 3 compare the curves calculated with the CNET model to the experimental data set of Yoshida and Matsumoto and Niimi [4,5], which covers the 900 - 1100°C temperature range. Although not corresponding to modern deep sub-micron technologies, this data set contains all the experimental features revealing the complex couplings between dopants and point defects, and is considered as a meaningful test for advanced diffusion models. As shown in Figures 1-3, the CNET model reproduces very nicely the features of the experimental profiles. In particular, thanks to the percolation effect, the model is able to account for the change in the shape of the profiles which occurs at high concentration. For intermediate concentrations, the simulated profiles exhibit the enhanced tail, with a more or less pronounced inflexion in the surface region. This inflexion is the result of the strong coupling between the defect gradients and the dopant, and its magnitude depends on the temperature: the lower the temperature, the stronger is the coupling, with a more pronounced inflexion as depicted by both the calculated and experimental curves. When the concentration exceeds about $2.5 \times 10^{20} \text{ cm}^{-3}$, the model is able to simulate both the formation of the plateau in the surface region and the strong tail enhancement resulting from the high point defect supersaturation generated by phosphorus diffusion. As illustrated in Figure 3 for the 1100°C (the same is true at the other temperatures), the standard full.cpl model fails to account for these experimental observations. Figure 2 shows also the simulated active concentration profiles. As observed experimentally, for the profile with the highest surface concentration, the calculated active concentrations are significantly lower than the total (chemical) phosphorus concentrations. In the CNET model this is due to the fact that the (dopant, defects) pairs have concentrations which are not negligible at high dopant concentration.

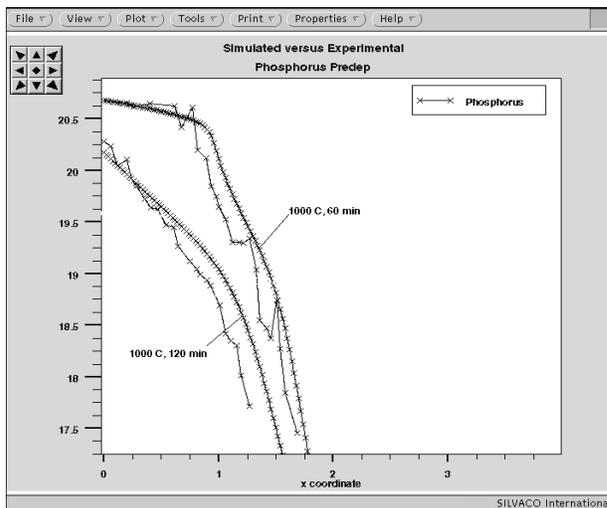


Figure 2. As in Figure 1, but at 1000°C. In addition, the simulated active P profiles are also plotted.

Finally let us comment on the CPU time used by this model. In fact the simulation time depends strongly on the conditions, and increases when the couplings between the point defects and the dopant become stronger (i.e. when a physical description of the diffusion requires this full model). Nevertheless, the CPU time remain quite reasonable. For example, on a SUN Sparc 10-40 workstation, the simulations reported on Figure 2 take about 13 min for the highest concentration (1 hour, 1000°C), and only 4 min for the lower concentration (2 hours, 1000°C). The same simulation (2 hours at 1000°C) requires less than 2 min if the surface concentration is decreased to $1 \times 10^{19} \text{ cm}^{-3}$ (intrinsic diffusion). This performances were obtained by using the "NEWTON" and "FULL.FAC" options in the "METHOD" statement.

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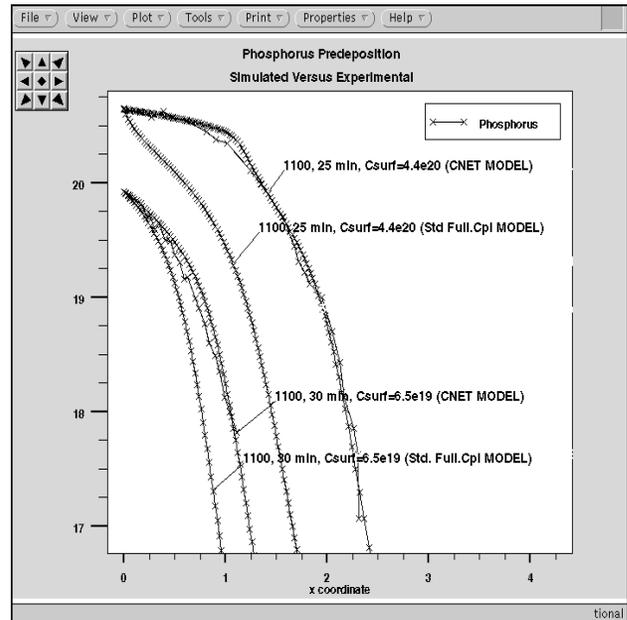


Figure 3. As in Figure 1, but at 1100°C. The results from the standard full.cpl model are also reported.