PEPPER - A Process Simulator for VLSI with a Non-Equilibrium Kinetic Diffusion Model

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SUMMARY

PEPPER is a program designed for advanced VLSI process simulation. The various features of the program are discussed, with particular emphasis on two new point defect models for diffusion. A general and flexible technique for rapid evaluation of new models has been implemented.

EXTENDED ABSTRACT

The trend in VLSI toward smaller device geometries has placed a greater demand on process simulation tools. This paper describes PEPPER, a simulator designed to allow the user to rapidly evaluate and implement advanced process models. PEPPER includes modules for deposition, etch, ion implantation, diffusion, oxidation, and epitaxy. The ion implantation module includes a new efficient and accurate algorithm for a Monte Carlo calculation of ion trajectories. The diffusion module contains a heirarchy of models, including the standard model [1], dynamic clustering, polysilicon grain boundary diffusion, and point defect diffusion. The epitaxy model uses the Langer-Goldstein algorithm for surface flux and autodoping. For oxidation the modified Deal-Grove formula is used and the nodes moved to account for volume expansion. Interstitials are generated at the Si-SiO_2 interface during oxidation and the impurity diffusion is solved fully coupled to the point defects.

A new point defect model is introduced which extends our earlier work [2]. Assuming that an impurity only diffuses by combining with a defect, that the law of mass action applies, and that the total impurity concentration, C, is dominated by its substitutional component, the following equation can be derived:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left\{\frac{f_I D}{C_I^*}\frac{\partial C C_I}{\partial x}\right\} - \frac{\partial}{\partial x}\left\{\frac{Z f_I D}{C_I^*} C C_I \frac{\partial \ln n}{\partial x}\right\} + \frac{\partial}{\partial x}\left\{\frac{(1-f_I) D}{C_V^*}\frac{\partial C C_V}{\partial x}\right\} - \frac{\partial}{\partial x}\left\{\frac{Z (1-f_I) D}{C_V^*} C C_V \frac{\partial \ln n}{\partial x}\right\}$$

where C_V and C_I represent defect concentrations, * denotes an equilibrium value, f_I is the relative interstitialcy component, and Z denotes the charge state.

In addition to oxidation enhanced or retarded diffusion, these equations can model extrinsic effects. Fig. 1 shows phosphorus diffusion in an inert atmosphere. A supersaturation of interstitials generated by the nonlinear coupling of phosphorus and interstitial atoms is responsible for the kink and tail of phosphorus, as well as the enhanced boron diffusivity.

The partial differential equations are solved using the Numerical Method of Lines with the resulting system of stiff ODEs being integrated with the LSODI package [3]. Since there are many open issues regarding impurity diffusion, PEPPER uses a flexible technique for developing and evaluating new models. The program allows the user to construct a system of PDEs on the input deck from a previously defined suite of fundamental operators (f_{xx} , f_x , $k{\cdot}f$, etc.) and boundary conditions (Dirichlet, Neumann, and Mixed) [4] , and so to change the underlying equations in a model easily.

To thoroughly test PEPPER's ablility to handle large PDE systems, a multiple species nonequilibrium kinetic model for phosphorus is being implemented. Following the work of Yoshida [5] and Mathiot-Pfister [6], diffusion occurs solely by phosphorus pairing with defects in various charge states. Ionization, pair formation, and bimolecular generation-recombination are modeled:

$$V^r + e^- \leftrightarrows V^{r-1} \qquad P^+ + V^r \leftrightarrows P^+V^r \qquad V^0 + I^0 \leftrightarrows \langle 0 \rangle$$

where P^+ denotes substitutional phosphorus, V^r a vacancy in the r^{th} acceptor state, and there are corresponding equations for interstitials. The time evolution of the species is described by a

system of twelve drift-diffusion-reaction equations. The large number of equations is offset by their simplicity, with all diffusivities constant. Moreover, under various simplifying assumptions, the kinetic model subsumes a heirarchy of advanced diffusion models from the literature[6,2]. Preliminary results are shown in Fig. 2 where concentrations of V^-, $V^=$, P^+V^-, $P^+V^=$, I^-, P^+I^-, and P^+ for a 10 min predeposition are plotted.

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Figure 1

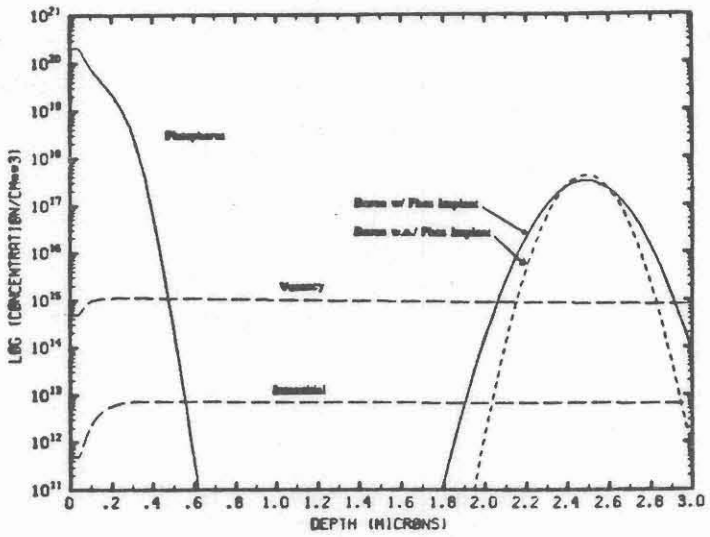

Fig. 1. Phosphorus implanted at $2\times10^{15}cm^{-2}$ 30keV and diffused for 60min at 900°C. The interstitial and vacancy concentrations become supersaturated, causing a tail in the phosphorus profile and enhancing the boron diffusion.

Figure 2

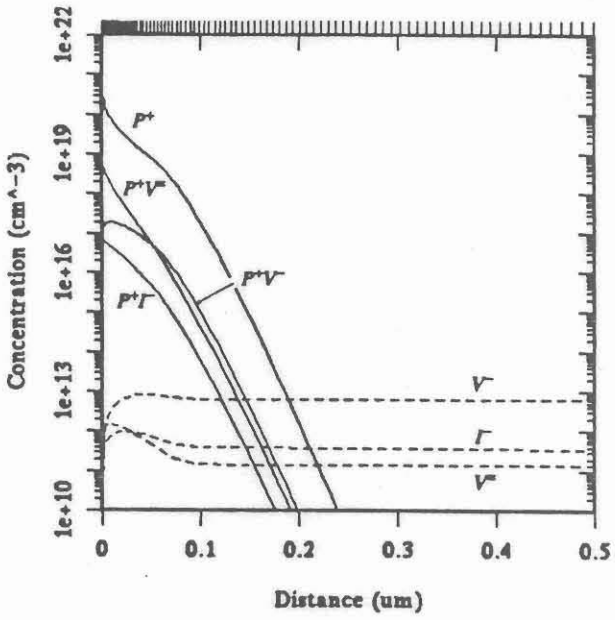

Fig. 2. A phosphorus predeposition at 900°C for 10min with a total surface concentration of $5\times10^{21}cm^{-3}$. The defect levels are perturbed from the equilibrium with acceptor states being dominant at the surface and a supersaturation of all defects observed in the bulk.