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Three-Dimensional Integrated Process Simulator : 3D-MIPS

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Abstract

We have developed a three-dimensional integrated process simulator of topography and impurity : 3D-MIPS. 3D-MIPS includes topography and impurity simulator, which can simulate deposition, etching, photolithography, BPSG flow, ion implantation, oxidation and impurity diffusion. The diffusion model, in particular, uses a novel equation which unifies diffusion and segregation. In this paper, these models and their simulation results are presented, and we demonstrate that it is possible to simulate 3D-complicated structures stably.

1. Introduction

Until now, three-dimensional (3D-) process simulators [1-3] have been developed. However, a 3D-process simulator which integrates topography and impurity has not yet been made. We have developed a new 3D-integrated process simulator(3D-MIPS: 3D-Mitsubishi Integrated Process simulator) of topography and impurity based on orthogonal mesh and mass-transport. The 3D-MIPS is a stable topography simulator with multiple-process steps using 3D-MULSS [4], and has recently implemented a impurity-diffusion model, an ion implantation model and an oxidation model. The diffusion model, in particular, has a novel equation. In this paper, these models and their simulation results will be presented, and we will demonstrate that it is possible to simulate 3D-complicated structures stably.

2. Models

2.1. Diffusion model

The diffusion model is based on the diffusion equation incorporating the electric field effect and Fair's vacancy model [5]. Neutral cluster model is used for boron, phosphorus, and antimony, and charged cluster model is used for arsenic. The used equation is described as follows:

$$\frac{\partial C_k}{\partial t} = -\nabla \cdot \boldsymbol{J}_k \tag{1}$$

$$\boldsymbol{J}_k = -\left(\frac{D_k}{m_k}\right)\nabla(C_k m_k) + Z_k a_k N_k E \tag{2}$$

$$m_k = \Pi_i {m_{ki}}^{\eta_i} \tag{3}$$

D_k : effective diffusion coefficient of impurity(No.k)
E : electric field
Z_k : the number of charges for impurity(No.k)
a_k : mobility of impurity (No.k)
N_k : concentration of active impurity (No.k)
m_k : segregation coefficient of impurity(No.k)
m_{ki} : segregation coefficient of impurity(No.k) for material(No.i)
η_i : volume rate of material(No.i) in a cell

I the right hand side of the equation (2), the first term corresponds to the new diffusion equation which is satisfied in both the inside of materials and the interface. The second term corresponds to the electric field effect.

As illustrated in Fig. 1, we assume that the impurity profile is continuous [6] and that there is a force moving the impurities in the interface of Si/SiO2. This force F can be given by the gradient of the external chemical potential difference: $\Delta\mu_{\text{ext}}$ between Si and SiO2. The flux density of diffusion can be derived from the Einstein relation and the relation between the segregation coefficient m and $\Delta\mu_{\text{ext}}$ [7] as follows:

$$\boldsymbol{J}_{\text{diff}} = -\left(\frac{D}{m}\right)\nabla(Cm) \tag{4}$$

Where the activity coefficients are assumed to be constant.

Within the Si and SiO_2 regions, m is constant and this equation becomes a normal diffusion one. We have, therefore, been able to obtain the unified equation of impurity diffusion which is satisfied in both the Si and SiO2 regions and the interfaces.

2.2. Implantation model

The implantation can deal with the impurities of boron, phosphorus, arsenic, antimony, and BF2. The depth profile is approximated by the Half Gauss or the PearsonIV distribution plus the exponential tail [6]. Then, by using the complementary error function, the depth profile is extended horizontally. The implantation to multiple layers is made possible by the respective stopping powers.

2.3. Oxidation model

The oxidation model was based on the 1-dimensional Deal-Grove model. The LOCOS structure is calculated by the horizontal extension using the Guillemot method [8].

2.4. Topography simulation model

We made a stable 3D-topography simulator with sequential steps by improving the algorithm of the 3D- topography simulator: 3D-MULSS [4]. The material surface is given by the equi-volume rate(0.5). The deposition model can deal with simple, isotropic, angle-dependent, Al-sputter, TiN-collimation sputter and plane depositions. The etching model can deal with simple, isotropic and anisotropic etching with mask-pattern and 2D-photo-image intensity, as calculated by Yeung method [9]. The BPSG flow is possible using the surface diffusion model [10].

3. Simulations

A simulation result of a LOCOS plus NMOS transistor structure is shown in Fig.2. The LOCOS structure was a two-dimensional simulation. 3D-ion implantations and 3D-diffusion were simulated by restarting from the 2D-LOCOS structure. The numbers of meshes are $30\times32\times60$. The most recent calculation time using CRAY-Y/MP was 4050 sec by improving upon the DeFault Frankel method. A DRAM cell structure of Quarter micron pitch was calculated and is shown in Fig.3. The mask data was transported from the lay-out editor via the online. There were 32 process steps, the analysis region was $0.8\times1.6\times2.4$ (μm), and the number of meshes were $20\times40\times60$. To date, the calculation time with CRAY-Y/MP is 3297 sec.

4. Conclusions

We have developed a three-dimensional integrated process simulator of topography and impurity : 3D-MIPS. 3D-MIPS has a 3D-topography simulator which can simulate deposition , etching, photolithography and BPSG flow, which in turn can calculate scores of sequential process steps in LSI's fabrication. The 3D-MIPS includes a new model which unifies the diffusion and the segregation models, the ion implantation model and the oxidation model. We have, thus, put forward the simulation results of LOCOS plus NMOS Transistor and DRAM cell structure of quarter micron pitch. In so doing, we have demonstrated that it is possible to solve the 3D-complicated structures stably.

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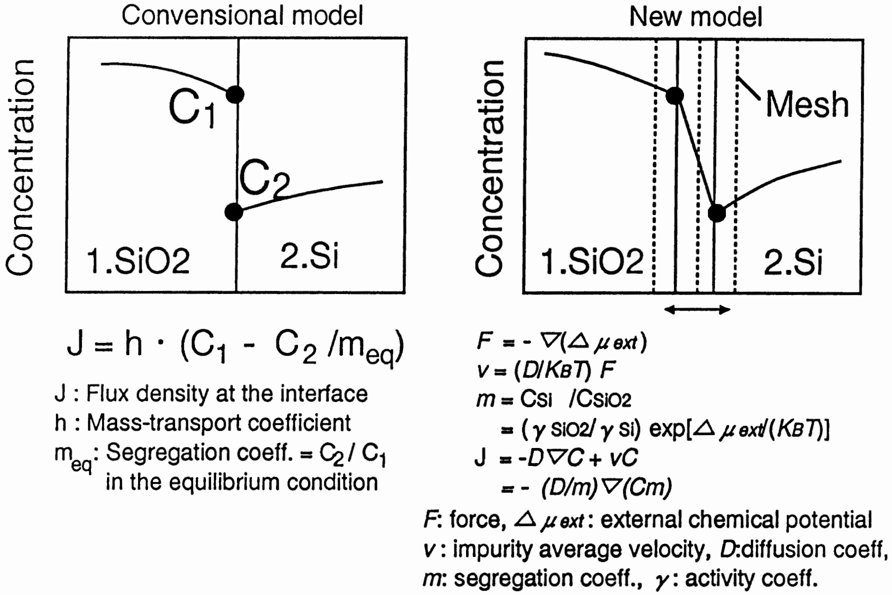

Fig.1 Model s of Diffusion and Segregation

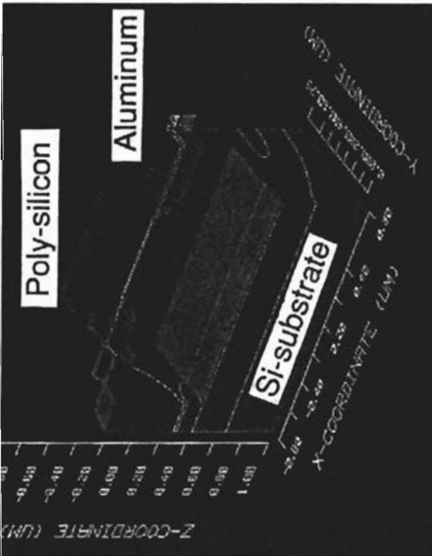

Fig.2 LOCOS + NMOS Transistor

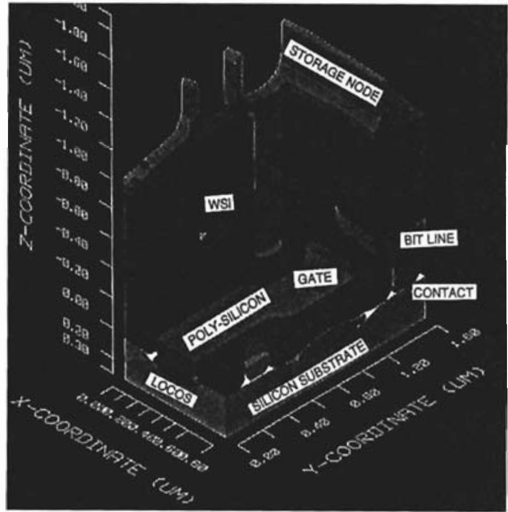

Fig.3 DRAM cell structure of quarter micron pitch