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Integration in the 2D Multi-layer Simulator TITAN of an Advanced Model for Dopant Diffusion in Polysilicon

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Abstract

A finite element formulation is proposed, based on the local homogenisation of polysilicon microstructure; the relevant physical phenomena considered during thermal treatment are the diffusion inside crystalline grains and along grain boundaries, segregation at grain boundaries and grain growth. This model has been successfully applied to the simulation of a bipolar device.

Diffusion in polysilicon is a complex phenomenon which can only be accurately modelled with a precise analysis of the polysilicon microstructure. A complete model has been established[1], which accounts for all phenomena involved in thermal annealing of polysilicon. It involves the diffusion of dopant inside the crystalline grains and along the grain boundaries, coupled with the displacement of grain boundaries due to grain growth. The columnar structure of the grains makes difficult the direct implementation of this model in a 2D simulator, particularly because the grain boundaries cannot all be perpendicular to the plane of the simulation. In the following, it is shown how a local homogenisation of the microstructure allows the diffusion in polysilicon and other layers to be simulated accurately, while avoiding the solving of a complex moving boundary problem.

1. Model main principles

Polysilicon is divided into small columnar crystalline grains separated by grain boundaries. The surfaces of the polysilicon layer are also grain boundaries. The dopants can be localised inside the crystalline grains, or at the grain boundaries. The grain structure is determined by the layer deposition conditions. However, this structure is modified locally by ion implantation, which amorphizes part of the polysilicon layer. Moreover, during thermal annealing, the size of the grain increases. The model includes the dopant concentration and temperature dependences of this grain growth. Dopants diffuse inside the grains according to the same laws as in silicon, whereas an enhanced diffusion occurs along the grain boundaries. At the grain boundaries, a segregation law links the grain boundary dopant concentration (C_{gb}, At/cm^2) to the grain interior dopant concentration (C_g, At/cm^3).

In order to implement this model in the 2D simulator TITAN[2], the division of the polysilicon layer into crystalline grains is replaced by two smoothly varying quantities: a vector function ($\vec{\xi}$) describing the main grain boundary orientation and the local density of grain boundaries (ρ_{gb}) representing the total area of grain boundaries per unit volume[3]. Only the surface of the polysilicon layer and interfaces with other materials are modelled explicitly as

grain boundaries. The quantities varying during dopant diffusion simulation are thus ρ_{gb} and, for each dopant, the concentrations C_{gb} and C_g. The grain growth is modelled by the evolution of ρ_{gb} during the annealing time, which depends on the local dopant concentration.

The dopants contained in the grain interior are assumed to diffuse isotropically, according to the same laws as in silicon. However, a full analysis of the 3D microstructure is necessary to determine and integrate the contribution of all grain boundaries (both normal to, and in the plane of, the 2D simulation) to the grain boundary diffusion in the plane of simulation. In the case of a square-based columnar structure, if $\vec{\xi}$ is in the plane of simulation, the resulting diffusion flux will thus be:

$$\vec{J}_{gb} = -D_{gb}\,\rho_{gb}\,[(\vec{\nabla}C_{gb}\cdot\vec{\xi})\,\vec{\xi} + \frac{1}{2}(\vec{\nabla}C_{gb}\cdot\vec{\eta})\,\vec{\eta}\,] \qquad (1)$$

where $\vec{\eta}$ is the unit vector perpendicular to $\vec{\xi}$ in the simulation plane, D_{gb} the diffusion coefficient of the dopant along grain boundaries.

Additionally to the diffusion fluxes, a segregation velocity has to be considered, coming from two different mechanisms: segregation by grain growth, and segregation by dopant diffusion. This velocity accounts for the fact that at the delocalised grain boundaries segregation conditions are established; it results in a source term coupling the evolution of grain interior and grain boundary concentration. At interfacial and surfacial grain boundaries, modelled explicitly, segregation is assumed between C_g and C_{gb}.

2. Discretisation

2.1 Diffusion equations

The spatial discretisation of the diffusion equations is finite element based. The elements are triangular. In the following, ϕ_i represents the base function associated to node i; the unknowns of the diffusion equations are:

at each node i inside a layer other than polysilicon: the concentration C^{ki} of each dopant k;

at each node i inside the polysilicon, for each dopant k: the grain interior concentration C_g^{ki} and the "volumic grain boundary concentration": $W_{gb}^{ki}=\rho_{gb}^{ki}\,C_{gb}^{ki}$;

At each node i of an interface (including the surface of polysilicon), for each dopant: the concentration in one of the materials or the grain interior concentration; the segregation conditions allows the determination of all other concentrations.

For stability purposes, an implicit scheme is used for the time discretisation. However, for the sake of simplicity, the time discretisation does not appear in the following equations. Consequently, the quantities appearing in the right hand side of the equations below have to be considered at time-step n, whereas the derivatives dC/dt must be understood as $(C_n-C_{n-1})/\Delta t_n$. According to this, the spatial formulation of the diffusion equation is, at each node i inside a non-polysilicon layer:

$$\int_{\Omega} \frac{dC^k}{dt} \phi_i \, d\Omega = \int_{\Omega} \vec{J}^k \vec{\nabla} \phi_i \, d\Omega \qquad (2)$$

where C^k is the restriction to the considered layer of the function $\Sigma C^{ki} \phi_i$; $\vec{J}^k$ is the flux of impurity k, which takes into account the concentration dependence of diffusion coefficients, and interaction between dopants: in silicon, $\vec{J}^k$ obeys a law in the form:

$$\vec{J}^k = -\sum_{k'} D^{kk'} \vec{\nabla} C^{k'} \qquad (3)$$

where $D^{kk'}$ depends on the concentrations of the dopants.

At a node i inside a polysilicon layer:

$$\int_{\Omega} \frac{dC_g^k}{dt} \phi_i \, d\Omega = \int_{\Omega} [\, \vec{J}_g^k \vec{\nabla} \phi_i - \rho_{gb}(q_1^k + q_2^k)\,(C_g^k - K^k C_{gb}^k)\, \phi_i \,] d\Omega \qquad (4)$$

$$\int_{\Omega} \frac{dW_{gb}^k}{dt} \phi_i \, d\Omega = \int_{\Omega} [\, \vec{J}_{gb}^k \vec{\nabla} \phi_i + \rho_{gb}(q_1^k + q_2^k)\,(C_g^k - K^k C_{gb}^k) \phi_i \,] \, d\Omega \qquad (5)$$

where q_1^k and q_2^k are the two components of the segregation velocity, as detailed below.

At a node at interface, or at the surface of polysilicon, the contribution of dopant diffusion inside the different material, and along the interfaces, have to be added:

$$\int_{\Gamma} \frac{dC_{gb}^k}{dt} \phi_i \, d\Gamma + \int_{\Omega} \frac{dC^k}{dt} \phi_i \, d\Omega = \int_{\Omega} \vec{J}^k \vec{\nabla} \phi_i \, d\Omega - \int_{\Gamma} D_{gb} \frac{\partial C_{gb}^k}{\partial \Gamma} \frac{\partial \phi_i}{\partial \Gamma} \, d\Gamma \qquad (6)$$

where Γ is the polysilicon boundary, C^k represents the total volumic concentration of impurity k (that is, in polysilicon, $C^k = W_{gb}^k + C_g^k$), $\vec{J}^k$ the volumic diffusion flux (in polysilicon, $\vec{J}^k = \vec{J}_{gb}^k + \vec{J}_g^k$). C^k is discontinuous at the interface, according to the segregation condition. The boundary integral in the right hand side accounts for the diffusion of C_{gb} along the interface.

Boundary conditions are in general homogeneous Neuman; however, Dirichlet conditions, or also non-homogeneous Neuman conditions can be considered in some cases (predeposition of dopant, oxide growth). They result classically either in the suppression of some degrees of freedom, or in boundary integrals not detailed here.

2.2 Grain growth

The grain growth follows equation 7:

$$\frac{dL_g}{dt} = K_g(\{C_g\} , \frac{L_g}{T_{poly}} , \frac{div\vec{\xi}}{L_g}) / L_g \tag{7}$$

where L_g is the grain diameter, inversely proportional to ρ_{gb}, K_g is the rate of grain growth which has a dependence on the grain doping concentration C_g, on the relative size of L_g to the layer thickness T_{poly} and also on the polysilicon layer curvature; this equation also determines the value of the segregation velocity component q_1^k:

$$q_1^k = \frac{1}{\alpha} \frac{dL_g^k}{dt} \tag{8}$$

where α is a dimensionless coefficient whose value lies between 1 and 2 depending on the exact dynamics of the grain growth[4]. This models the transport and segregation of dopant by a moving grain boundary.

The second component of the segregation velocity models the diffusion of dopant from grain interior to grain boundary:

$$q_2^k = \frac{D(C_g^k)}{2\,L_g} \tag{9}$$

where D is the grain diffusion coefficient. Both q_1 and q_2 are dopant dependent.

2.3 Solving

At each time step, the grain growth (equation 7) is first solved at each node; the grain boundary density $\rho_{gb}{}^i$ and the segregation velocities ($q_1{}^{ki}$, $q_2{}^{ki}$) are determined, according to equations 8 and 9. Then, the set of diffusion equations (2,4,5,6), added to the segregation conditions at interfaces, is considered. For stability purposes, an implicit scheme is used.

The first approach to solving the diffusion equations employed a SOR method, where the diffusion coefficients were recomputed at each iteration. This method has the advantage of a very poor memory requirement, and is quite efficient in the case of classical diffusion equations, with a mesh size adapted to the diffusion coefficients. However, in polysilicon, the discrepancy between the diffusion coefficients in grain interior and in grain boundaries, added to the necessity of a thin mesh near the interfaces, force the mesh size to be very small, when compared to the diffusion coefficient in grain boundaries. The SOR method becomes thus very inefficient (more than 100 iterations at each time-step).

In a more recent approach, the non-linearity resulting from the dopant dependency of the diffusion coefficients (in silicon and in polysilicon grains) can now be solved either by SOR, or by successive Newton iterations, where the linear solver is conjugate gradient. Of course the memory requirements are much higher in the latter case, especially because the number of coupled unknowns at each node of the polysilicon is twice the number of dopants. In a realistic problem like the one presented below, with 3 dopants diffusing simultaneously and around 2000 nodes, the size of the matrix is quite big. However, as far as CPU time and results

accuracy are concerned, the Newton algorithm brings a comfortable gain in the case of polysilicon.

3. Application

The program has been applied to the simulation of a bipolar transistor. The emitter and base contact regions are formed by out-diffusion from polysilicon layers. Figure 1 shows the final geometry and dopant distribution as simulated by TITAN-POLY. Figure 2 shows the grain direction at each node of the polysilicon layers. Figure 3 shows the mesh used for the simulation. Figure 4 compares the 1D vertical simulated profile through the emitter base with measured SIMS profiles. The total CPU cost of this simulation is around 15mn on a CONVEX 220.

Conclusion

With the application of local homogenisation of the polysilicon microstructure, accurate simulation of dopant diffusion and grain growth in non planar polysilicon layers is possible in a 2D process simulator. An efficient numerical implementation, through finite element discretisation of the coupled diffusion equations, has been presented. The application of this model to the simulation of an advanced bipolar transistor has been demonstrated. The general approach presented here has potential application to diffusion problems in other polycrystalline materials.

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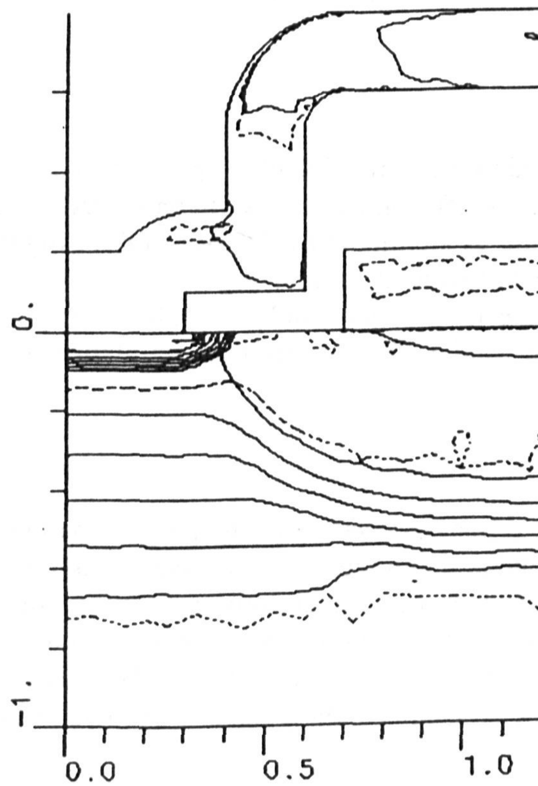

Figure 1: The geometry and dopant contours in the active region of a 1 μm double polysilicon bipolar device simulated by TITAN-POLY. The base contact was formed by boron out-diffusion from the p-poly layer; the emitter by arsenic out-diffusion from the implanted n-poly layer during an RTA at 1100 C.

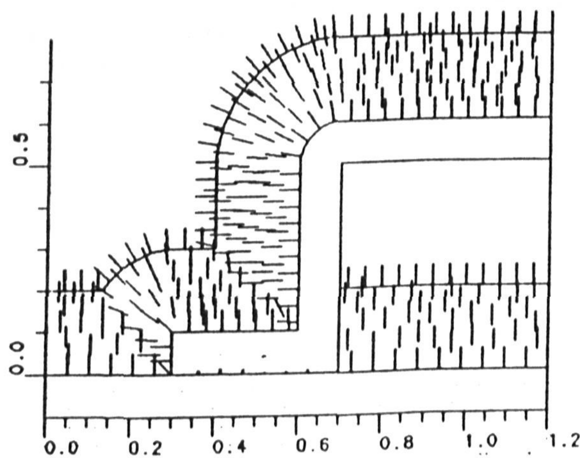

Figure 2: The grain direction $\vec{\xi}$ considered at each node of the polysilicon layers, in the device shown in Figure 1.

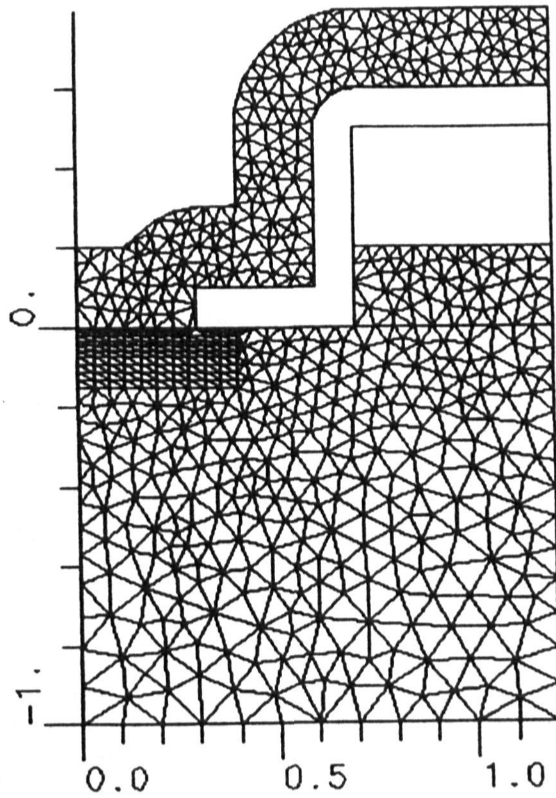

Figure3: The mesh used for the simulation of the bipolar transistor shown in Figure 1.

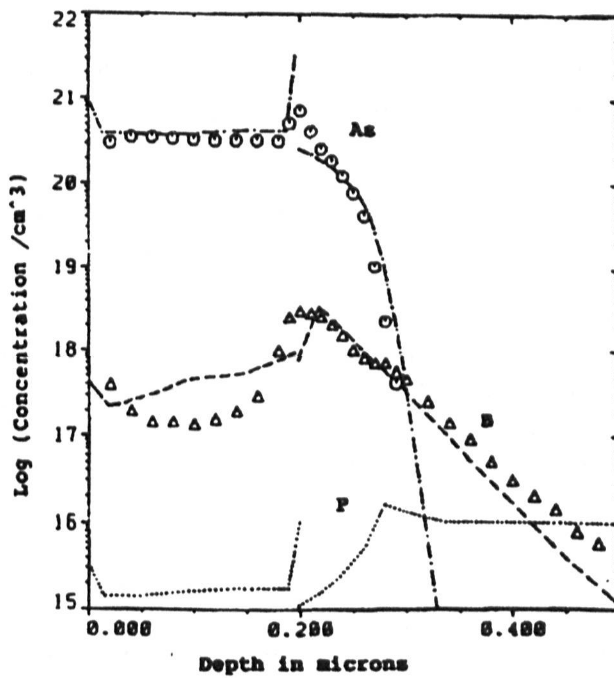

Figure 4: The vertical arsenic and boron simulated profiles through the emitter-base region of the device shown in Figure 1 are compared to experimental SIMS data. The boron was implanted through dielectric screening layers.