A Two-Dimensional Process Model for Silicide Growth

C.M.Li, T.Crandle, M.Temkin, and P.Hopper
SILVACO International, 4701 Patrick Henry Dr., Bld.3, Santa Clara, CA 95054
Telephone (408)-988-2862, Fax (408)-988-3285

Computer modeling of silicide growth[1] [2] is useful for predicting silicide thickness and the diffusion dopants inside the silicide. With scaling to submicron dimensions and polycide/salicide technology development, computer models capable of handling complicated geometrical movements of multi-layer materials, coupled with defects injection and impurity redistribution at the moving interfaces or inside the material layers, will become more useful in the development of improved silicide processes. A two- dimensional numerical silicide model has been developed to address these problems. It is implemented in SSUPREM4[3], a general 2D process simulator. The model accounts for movements of metal-silicide and poly/silicon-silicide boundaries and chemical reactions between silicon and metal atoms which take place at the boundaries. The moving boundary velocities are calculated using the interface reaction rate coefficients and the concentrations of silicon and metal in the silicide. The diffusion of silicon and metal atoms inside the silicide layers are solved using point defect diffusion equations. Impurity segregation and diffusion in silicide are included, as well as point defect injection from the moving interfaces. The user defined material capability of SSUPREM4 allows multiple material combinations to be defined for specific applications.

The movement of each silicide interface is coupled with the impurity/defect diffusion in way that is analogous to that used to describe oxidation. During each time step, and for each interface point, the growth velocities are calculated based on the temperature, the surface reaction rate coefficients, and the silicon/metal concentrations. The velocities are then used as the boundary conditions for solving diffusion equations for silicon/metal together with other impurities. The resulting concentration distribution is used to calculate the interface velocity at the next time step. For the ith interface point, the growth velocity is calculated as

$$\frac{dX_i}{dt} = k_i \; C_i \; n_{in} \; / \; N_{1i} \qquad (1)$$

where k_i is the interface reaction rate coefficient, N_{1i} is the number of silicon or metal molecules per unit silicide material, C_i is the silicon or metal concentration at the silicide side of interface, and n_{in} is the interface normal vector pointing towards the silicon/poly or metal side.

The diffusion of silicon and metal molecules inside the silicide layers is modeled as a point defect diffusion process, where the silicon and metal can react to form the silicide, similar to the recombination of interstitials and vacancies.

$$\frac{\partial C}{\partial t} = \nabla \; (D \; \nabla C \;) \; - R \qquad (2)$$

where C is the concentration of either silicon or metal molecules, R is the bulk recombination of silicon and metal molecules, and D is the diffusivity of silicon/metal inside the silicide. When diffused silicon/metal flux reaches the growth interface, part of the flux will take part in the interface chemical reaction to form the silicide. Another part of the flux can diffuse across the boundary into the silicon/poly or metal layers, so in addition to bulk recombination, segregation and transport coefficients are used as the boundary conditions to describe the sinking drain of diffused silicon/metal molecules.

Silicide formation usually leads to a large volume decrease, which is one of reasons for the stress observed in the material. The volume change associated with an interaction is modeled using atomic volumes of the reacting species and molecular volume of the reacted product[4]. For a reaction of the type $x\ M + y\ Si \rightarrow M_x\ Si_y$ the change ΔV (%) is given by

$$\Delta V = \frac{(x \; V_M + y \; V_{Si} \;) \; - V_{M_x Si_y}}{x \; V_M + y \; V_{Si}} \times 100 \qquad (3)$$

where $\Delta V, V_M, V_{Si}$, and $V_{M_x Si_y}$ are the percentage molecular volume change, the molecular volume for metal, silicon and silicide respectively, and x and y are the number of metal and silicon atoms in the silicide $M_x Si_y$.

The two-dimensional movement of growth interface and volume change induces stress in formed silicides, causing viscous flow of silicide layers. This silicide flow is modeled in analogy to the compress model of oxidation, where a

set of creeping equations are solved to determine the velocity distributions in the floating silicide layers [5]

As an example, simulation has been performed of a Titanium salicide process at $700^o C$ for 10 min. The calculated results indicate that silicide layers extend from poly gate and source contact into the oxide spacer. This is in agreement with the experimental results presented by Osburn et. al. [6]. Adjustment of temperature, time and other diffusion parameters allows the bridging problem of salicide process to be simulated. Also plotted are the velocity and silicon interstitial distributions. The shrink of silicide volume results in a distortion of oxide spacer shape.

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