Moving Boundary Applications in Process and Interconnect TCAD

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Modern Technology Computer Aided Design (TCAD) applications demand mathematical descriptions of physical phenomena, which are both accurate and suitable for numerical implementation. In the case of an evolving surface, mathematical models include material exchange between surface and surrounding phases and, at the same time, material transport along the surfaces. Stress phenomena often play a crucial part in the formation and evolution of free surfaces and, therefore, a model framework must also consistently include mechanical sub-models. For some applications, such as simulation of crystalline texture evolution, it is also necessary to extend the single surface models towards surface models for multiphase systems.

The numerical handling of mathematical models has to produce computationally efficient algorithms with reasonable demand on computer resources. Convergence and stability conditions should not impose strong restrictions on the choice of simulation domain geometries and discretization meshes.

The most general form of an evolving surface normal speed $v_n(\mathbf{r})$ used in TCAD applications is

$$v_n(\mathbf{r}) = \nabla_s(D(\mathbf{r})(q\mathbf{E}(\mathbf{r}) + \gamma_s\Omega\nabla_s\kappa)\cdot\mathbf{t}) + F(\mathbf{r}). \tag{1}$$

The first term corresponds to surface material transport which is driven by the external field ($\mathbf{E}(\mathbf{r})$) and the curvature gradient ($\nabla_s\kappa$). $D(\mathbf{r})$ is the anisotropic surface diffusivity, $\mathbf{t}$ is the unit vector tangential to the surface, γ_s is the surface

energy, Ω is the volume of an atom, q is the effective charge, and $F(\mathbf{r})$ is the general speed function depending on the material exchange with the surrounding phases. Equation (1) describes the motion of a sharp interface, which implies that any utilized numerical approach has to deal with spatial discretization of an evolving surface. The surface is described by specifying a usually large number of points on it. Over the time the phase surface evolves and changes its morphology and even more points may be required to accurately describe it. Such techniques are quite complicated to implement and also tend to have rather poor numerical stability.

For the investigation of electromigration induced void evolution we have applied a modified Chan-Hilliard equation [2, 1]. Here, the dominant material transport is electromigration and self-diffusion at the void surface. A material exchange between a metal bulk and the void surface is neglected so that the sharp interface formulation of the moving boundary given by (1) can be simplified by setting $F(\mathbf{r}) \equiv 0$. The Chan-Hilliard theory enables a representation of an evolving void surface as interface between two phases. Both phases are defined by values of an order parameter ϕ, which takes the value $+1$ in the metal and the value -1 in the void area. This interface between phases is not sharp but has a finite width where ϕ takes values between -1 and $+1$. The phase field interpretation of the model equation (1) is

$$\frac{\partial \phi}{\partial t} = \frac{2D}{\epsilon \pi} \nabla \cdot (\nabla \mu + q\mathbf{E}), \tag{2}$$

$$\mu = \frac{4\Omega\gamma_s}{\epsilon\pi}(f'(\phi) - \epsilon^2 \Delta\phi). \tag{3}$$

where μ is the chemical potential, $f(\phi)$ is the double obstacle potential as defined in [1], and ϵ is a parameter controlling the void-metal interface width. The equation system (2),(3) is solved by means of a finite element method in combination with adaptive mesh refinement [2]. The described approach is utilized for investigation of void behavior in the vicinity of high gradient electrical fields and void collision with a barrier layer [2].

During deposition or etching in process technology a material is added or removed from the free evolving surface, respectively. A general assumption is low adatom mobility so that the first term in (1) can be neglected and the surface evolution is defined by the simple relation $v_n(\mathbf{r}) = F(\mathbf{r})$. The speed function is generally related to properties of the reactor, where the deposition or etching process takes place. In this case it is convenient for simulation to apply the Level Set method [4]. This approach is presented considering as an example the etching of sacrificial silicon dioxide (SiO_2) layer by hydrofluoric acid (HF).
The chemical reaction on the surface of the sacrificial layer is [3]

$$6\,\mathrm{HF} + \mathrm{SiO_2} \longleftrightarrow \mathrm{H_2SiF_6} + 2\mathrm{H_2O}. \tag{4}$$

The transport of the etching agent (HF) occurs via linear diffusion,

$$\frac{\partial C_{\mathrm{HF}}}{\partial t} = \nabla \cdot (D \nabla C_{\mathrm{HF}}), \tag{5}$$

with the boundary conditions $C(0,t) = C_b$ where the etching agent enters the simulation domain. On the interface between the sacrificial layer surface and the etch medium (etching front) the following boundary relationships hold

$$\begin{aligned} C_{\mathrm{HF}}(\mathbf{r},t) &= C_s, \\ \frac{\partial C_{\mathrm{HF}}}{\partial \mathbf{n}} &= J_{\mathrm{HF}} = k_1 C_s + k_2 C_s^2, \end{aligned} \tag{6}$$

for $t > 0$. $\mathbf{r}$ is the position vector belonging to the etching front and $\mathbf{n}$ is the normal vector.

The geometrical shape of the etching front is described by the Level Set function ϕ. The zero iso-surface is equivalent to the geometrical interface. The Level Set function has a same meaning as order parameter in Chan-Hilliard theory and therefore the same symbol ϕ is used. For a given speed function F the governing equation of the Level Set is [4],

$$\frac{\partial \phi}{\partial t} + F\|\nabla\phi\| = 0. \tag{7}$$

On the basis of equation (4) we obtain the characteristic speed function for sacrificial etching at the etching front,

$$F = -\frac{\Delta\delta}{\Delta t} = -6\, J_{\mathrm{HF}}\, \frac{1}{\rho_{\mathrm{SiO_2}}}, \tag{8}$$

where $\Delta\delta$ is a small displacement of the etch front during time step Δt. This locally determined speed function is extended to the whole simulation domain in order to solve equation (7). The relationships (6) can now be rewritten to include the Level Set description of the etching front. Introducing a parameterized surface description $\mathbf{r}_\phi = \mathbf{r}_\phi(\alpha_1, \alpha_2)$, where $\alpha_1, \alpha_2 \in R$ and are chosen so that $\phi(\mathbf{r}_\phi) = 0$, leads to

$$\begin{aligned} C_{\mathrm{HF}}(\mathbf{r}_\phi,t) &= C_s, \\ \frac{1}{\|\nabla\phi\|}\nabla C_{\mathrm{HF}} \cdot \nabla\phi\Big|_{\mathbf{r}=\mathbf{r}_\phi} &= J_{\mathrm{HF}} = k_1 C_s + k_2 C_s^2. \end{aligned} \tag{9}$$

By means of equations (5) and (7) and the interfacial conditions (9) the moving boundary problem is well-defined. Simulations based on this model are used for investigations of a sacrificial layer profile in dependence on an etch agent distribution.

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References

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