Anisotropic Laplace Refinement for Three-Dimensional Oxidation Simulation

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Abstract

We present a computational method for three-dimensional tetrahedral mesh refinement according to the demands of oxidation simulation. The main focus lies on two major problems. First, the start-up condition of oxidation claims an initial mesh preparation which is done by the so called Laplace refinement, second the transient conversion of silicon (Si) to silicon dioxide (SiO_2) forces a high spatial resolution in a small area around the material interface which shows the need of adaptive refinement on demand. More over our approach takes anisotropy into account to keep the amount of elements small compared to strict isotropic refinement.

1 Introduction

Oxidation, by the means of a process step involved in the fabrication of integrated circuits (IC), is an directional and surface near process step. This means that the interesting simulation region is near the surface and therefore it is important to guarantee a good spatial resolution at the *skin* of the simulation domain.

This can only be achieved efficiently by anisotropic meshes. Strict isotropic three-dimensional regular meshes are not practicable for realistic structures due to required high resolution compared to the size of the simulation domain. The demand on calculation time and the limitation of memory requires anisotropic meshes.

The generation of small, strongly anisotropic, and unstructured mesh layers by three-dimensional mesh generators is, unfortunately from a technology point of view, still something of an art, as well as a science [1]. A more robust way is to generate mostly isotropic coarse initial meshes for instance with a Delaunay mesh generator, followed by a mesh adaption post processing step on demand. A means to an end for this task is a robust grid refinement step which is based on tetrahedral bisection. One way to increase spatial resolution and to take anisotropic mesh refinement at the same time into account was shown in [2]. The basic idea in this work is to introduce a metric tensor function. The initial mesh refinement is based on the solution of the Laplace equation, while the dynamic adaptation observes the diffuse interface function which describes the moving boarder between silicon and silicon dioxide.

2 Anisotropic Metric

The idea used in our approach is to apply a combination of rotation and dilation to define an anisotropic metric. The dilation is represented by three scalar values $\lambda_\xi, \lambda_\eta$ and, λ_ζ, respectively. Using $(\vec{\xi}, \vec{\eta}, \vec{\zeta})$ and $(\lambda_\xi, \lambda_\eta, \lambda_\zeta)$ we define two matrices

$$\mathbf{R} := \begin{pmatrix} \xi_x & \eta_x & \zeta_x \\ \xi_y & \eta_y & \zeta_y \\ \xi_z & \eta_z & \zeta_z \end{pmatrix} \text{ and } \mathbf{S} := \begin{pmatrix} \lambda_\xi & 0 & 0 \\ 0 & \lambda_\eta & 0 \\ 0 & 0 & \lambda_\zeta \end{pmatrix} \text{ which leads to } \mathbf{M} := \mathbf{R}\mathbf{S}\mathbf{R}^T. \quad (1)$$

The anisotropic metric $\mathbf{M}$ is a tensor function which varies over the domain $\mathbf{M} = \mathbf{M}(x, y, z)$. The tensor function is symmetric and positive definite which allows to use this tensor as a metric tensor.

3 Laplace Refinement

Our idea is to use the solution of Laplace's equation as approximation for a surface distance function. The imagination is based on electrostatic field calculations of the plate-capacitor. A typical plate-capacitor structure is formed by two coplanar metal planes which are connected to a voltage supply. We neglect the surrounding area by applying zero Neumann boundary conditions at open borders of the capacitor and Dirichlet boundary conditions at the electrodes (assumes an infinitely expanded capacitor). Iso-surfaces of the electrostatic potential inside the plate-capacitor form also coplanar planes which can be used as a measure for the perpendicular distance to the surface (electrodes).
For the description of the metric tensor function, we first calculate the solution of Laplace's equation considering the given Dirichlet boundary conditions on the initial coarse mesh. This approach allows to define in a very flexible way where the refinement should take place. To take anisotropy into account we use the derivative of the electrostatic potential ψ as primary stretching direction for the anisotropic metric description (1). To accomplish this task we first rotate the three axes of the Cartesian coordinate system (x-, y-, and z-axes) so that the *new* y-axis is parallel to the gradient vector $\nabla\psi$.
At the second step we apply a dilation-factor-function $\lambda_\eta = \lambda_\eta(\psi)$. So the dilation along the gradient direction depends on the potential ψ. All other stretching weights are set to unity, which guarantees a dilation only along the gradient field. According to (1) the anisotropic metric function is now completely specified over the element. For the three-dimensional simplex partitioning the *anisotropic length* of all tetrahedron edges are calculated under consideration of

$$\ell_{PQ} = \int_0^1 \sqrt{\overline{PQ}^T \cdot \mathbf{M}(P + t \cdot \overline{PQ}) \cdot \overline{PQ}}\, dt. \quad (2)$$

The longest anisotropic edge which transcends the maximum edge length value is chosen as the refinement edge.

4 Oxidation

For the oxidation model we use analogously to [3, 4] a normalized silicon concentration $\eta(\vec{x},t) = \frac{C_{Si}(\vec{x},t)}{C_{0Si}}$ where $C_{Si}(\vec{x},t)$ is the silicon concentration at time t and point $\vec{x}(x,y,z)$ and C_{0Si} is the concentration in pure silicon. So η is 1 in pure silicon and 0 in pure silicon-dioxide. The oxidant diffusion is described by $D\Delta C(\vec{x},t) = k(\eta)C(\vec{x},t)$. Here D is the diffusion coefficient and $k(\eta)$ is the strength of a spatial sink and not just a reaction coefficient at a sharp interface like in the standard model for oxidation [5]. However, $\eta(\vec{x},t)$ varies during oxidation simulation with ascending time, so therefor it is important for the convergence of the model and the quality of the computed solution to increase the spatial resolution near the interface on demand.
The idea is to solve the Laplace equation on the initial coarse mesh with special Dirichlet boundary conditions. Boundary conditions on the upper silicon surface which is exposed to an oxidizing atmosphere are set to unity and the opposite part of the silicon body is set to zero. The solution of the Laplace equation and the corresponding isosurfaces can be seen in the right part of Figure 1, the initial coarse mesh is shown in the left part. For the refinement post processing step we detect those elements which hold a solution value close to unity, all others are untouched. The orientation of the anisotropy should reflect boundary aligned elements by the mean of short point distances perpendicular to, and long point distances along the oxidizing surface. Observing the gradient field of the solution, c.f. Figure 1(b), reflects the anisotropic compression direction and is therefore a good choice for the anisotropic tensor function.
While performing the simulation we use $\eta(\vec{x},t)$ to identify the interface region and the first derivative of η for our anisotropic refinement. Figure 2(b) shows the resulting mesh at the end of the oxidation simulation caused by applying our strategy. The interface between silicon and silicon dioxide migrates from the upper surface of the initial silicon body downwards. The refinement procedure follows this behavior and thereby a good spatial resolution near the interface is reached. Other regions at the simulation domain are left untouched which guarantees the usage of an almost minimal number of grid points.

References

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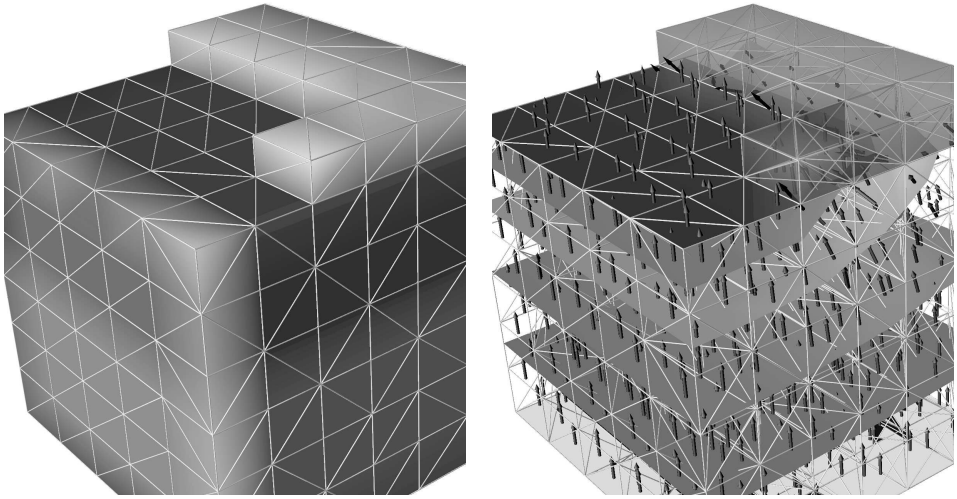
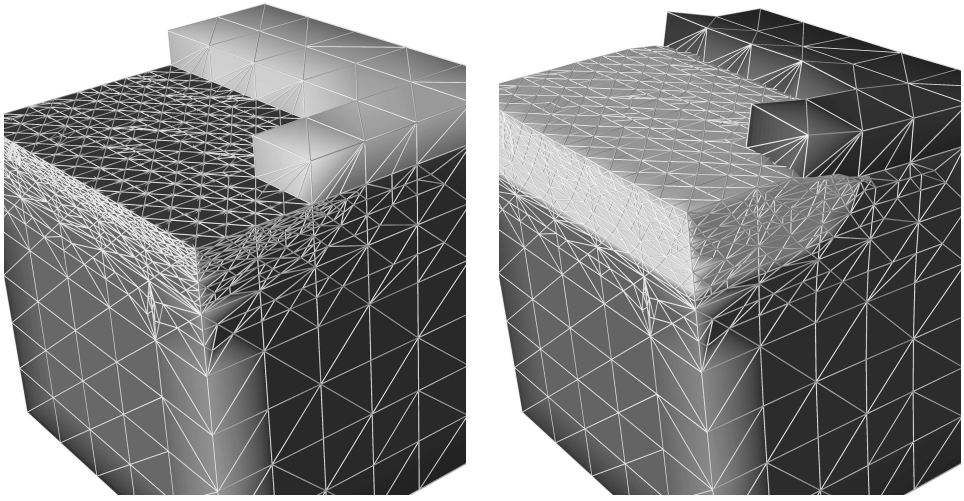


(a) Cubic silicon (Si) body with L-shaped silicon nitride (Si_3Ni_4) mask on top. Initial mostly coarse regular mesh.

(b) Iso-surfaces of Laplace's equation solution and according gradient field vectors on initial coarse mesh.

Figure 1: Calculations for anisotropic refinement on the initial coarse mesh.



(a) Highly anisotropic thin mesh layer after Laplace-Refinement in the upper region of the silicon body (input for oxidation).

(b) Anisotropic mesh after oxidation simulation. The refinement procedure followed the moving interface of Si and SiO_2.

Figure 2: Mesh adaption during oxidation simulation.