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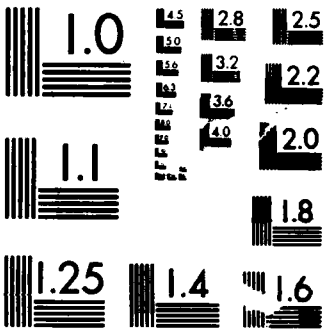

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A VISCOELASTIC BEM FOR MODELING OXIDATION

Thye-Lai Tung, Jerome Connor, and Dimitri A. Antoniadis

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A viscoelastic boundary element method has been developed to model the motion of silicon dioxide and silicon nitride during thermal oxidation of silicon. This technique uses Kelvin's solution reformulated according to the correspondence principle on viscoelasticity. Constant velocity loading is chosen to ensure smooth variations in displacement and stress behavior for a wide range of relaxation times.

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Abstract

A viscoelastic boundary element method has been developed to model the motion of silicon dioxide and silicon nitride during thermal oxidation of silicon. This technique uses Kelvin's solution reformulated according to the correspondence principle on viscoelasticity. Constant-velocity loading is chosen to ensure smooth variations in displacement and stress behavior for a wide range of relaxation times.

1 Introduction

A major problem in modeling thermal oxidation of silicon is the moving boundaries. Driven by the conversion of silicon to silicon dioxide of increased volume, boundaries change shape drastically during a local oxidation of silicon (LOCOS) process step. Conventional methods such as the finite element method (FEM) require a mesh to subdivide the simulation domain. To apply such methods to thermal oxidation, one must first develop computer codes to regenerate the mesh automatically and optimally as the oxide changes shape at every time step [1,2,3]. After that, one may have to deal with the transfer of stress history from the old mesh to the new one, depending on what oxide flow model is used. This is another difficult problem if one wishes to minimize numerical diffusion of stress distribution due to regriding.

In contrast to the FEM, the boundary element method (BEM) does not require a mesh in general since it does all calculations on the boundary but not in the interior. Because segments need not be regenerated, keeping track of stress history on the boundary is straight forward. However, previous efforts on applying the BEM to model oxide motion as viscoelastic flow suffered from some drawbacks. In Matsumoto's formulation [4], domain calculations were needed. Although restrictions on the grid were not as stringent as those in the FEM, excessive computation time was evident. Simulation setup might still be difficult for complex structures. Isomae attacked the problem differently by using a Laplace transform technique [5]. According to the correspondence principle of linear viscoelasticity, we may solve a viscoelastic problem through an equivalent elastostatic system in the Laplace transform space. Boundary element techniques for elastostatics do not require domain calculations, but unfortunately it is impossible to solve Laplace transforms analytically in any practical simulation situations. Numerical Laplace transform, as used

by Isomae, is deemed wasteful because a new solution must be generated at every time step.

In this paper we describe a generalized BEM for two-dimensional linear viscoelastic flow, with application to thermal oxidation. Instead of performing the Laplace transform on the global solution, we operate it on the fundamental equations. Our kernel functions are derived from Kelvin's solution used in elastostatic BEM applications [6]. A suitable excitation function is added to produce a time-varying body force that causes the load point to move with a constant velocity in a viscoelastic medium. This approach eliminates domain calculations and numerical Laplace transforms. Yet, it is as easy to use as those for elastostatics. The main disadvantage is that boundary conditions cannot be satisfied for all times, so the system must be solved periodically. But that is not a problem for thermal oxidation because a new solution must be obtained anyway for every time step. This formulation can handle all possible values of Poisson's ratio and a wide range of stress relaxation times, essentially encompassing viscous incompressible flow and elastic deformation.

2 Numerical Formulation

We implement the viscoelastic BEM using the so-called indirect formulation, which is also known as the classical or source method. Here we attempt to model a problem by putting "sources" on the boundary and adjust their strength so that the fields they generate match the prescribed boundary conditions. For a potential problem, the sources are simply electrical charges. The indirect formulation has an advantage over the direct formulation in that different components within the stress tensor or displacement vector can be obtained more readily.

The thermal oxidation process actually consists of two tightly coupled processes, namely oxidant diffusion, and oxide motion. For details on the oxidant diffusion process, boundary conditions, and numerical implementation of the integral equations, readers are referred to our previous paper on the same subject [7]. In that paper we use an incompressible viscous flow model for oxide motion; here we have a generalized model applicable to the oxide, silicon nitride and silicon substrate.

The two sets of integral equations for viscoelasticity are shown below:

$$\sigma_{ij}(\vec{x}) = \int_\Gamma \rho_k(\vec{\xi})\sigma^*_{ijk}(\vec{x}-\vec{\xi})\mathrm{d}\Gamma$$

$$u_i(\vec{x}) = \int_\Gamma \rho_j(\vec{\xi})u^*_{ij}(\vec{x}-\vec{\xi})\mathrm{d}\Gamma$$

where σ_{ij}, u_j, and ρ are the stress tensor, displacement vector, and source density respectively. Γ denotes the boundary. σ^*_{ijk} and u^*_{ij} are the kernels; their actual forms are given in the appendix. For compactness, Einstein notation has been used. To get the surface traction, we apply the following formula:

$$p_i(\vec{x}) = \sigma_{ji}(\vec{x}) n_j(\vec{x})$$

where n_j is the direction cosine of the surface.

If we want to treat silicon nitride as an elastic material with stiffness, we have to modify the boundary condition of the oxide-nitride interface from a free surface condition $\vec{p} = 0$ to the following:

1. displacement vector is continuous across the interface,

2. surface tractions of the two materials are equal and opposite.

To ensure stability, the equations for silicon nitride layer and oxide region must be solved simultaneously. The resulting system matrix is larger but banded.

Likewise, we use the same approach if we desire to model the silicon substrate as an elastic foundation, instead of treating it as a rigid body. Note that due to the unique formulation of BEM, boundary conditions at $y = -\infty$ need not be specified for the silicon substrate.

In viscoelasticity, we must include past stress history in the present time step. Consider p^m_n, the normal component of the surface traction at time step m. The two different relaxation terms, as defined in the appendix, are kept seperated and updated in the following way:

$$\begin{aligned} p^m_{n\alpha} &= p_{n\alpha} + p^{m-1}_{n\alpha} \exp(-\Delta t^m/\tau_\alpha) \\ p^m_{n\beta} &= p_{n\beta} + p^{m-1}_{n\beta} \exp(-\Delta t^m/\tau_\beta) \end{aligned}$$

where Δt^m is the time step size, τ_α and τ_β the characteristic relaxation time constants.

3 Simulation Results

We will demonstrate how stress is relieved via viscoelastic flow, the effect of the silicon nitride layer on the oxide shape and the stress distribution. The relaxation time, or equivalently the viscosity, of oxide has not been determined accurately. It is diffucult to do so because, for a given temperature, the viscosity depends on the quality of the oxide, water contents, and the presence of other impurities. Most of the recent data on oxide

viscosity are inferred rather than measured directly in experiments, but they are useful as ballpark figures. In any case, it is a good exercise to vary the relaxation time to see how it affects the stress distribution.

Shown in Fig. 1 is the outline of a semi-recessed LOCOS structure plotted for every time step. In this simulation window of 1.6μm wide, the silicon nitride mask extends from $x = 0$ to $x = 0.96\mu$m and is assumed to be totally flexible. Initially the structure has a pad oxide thickness of 200Å. Oxidation is carried out at 925°C in a wet ambient for 3.4 hours to get a final field oxide thickness of 5000Å. The Young's modulus and Poisson's ratio are taken to be 8×10^{11} dynes·cm^{-2} and 0.194. Shown in Fig. 2a, 2b and 2c is the normal surface traction at the oxide-silicon interface corresponding to relaxation times ($\frac{\eta}{G}$) of 100 hours, 1 hour, and 1 minute respectively. The normal component of the surface traction is plotted for every time step, just like the outline of the oxide in Fig. 1. (Because the oxide shape is almost identical for all relaxation times, only one is shown in Fig. 1.) In all the 3 stress plots, there are two peaks in the compressible stress region (negative value range). The early peak occurs at the edge of the nitride mask ($x = 0.96\mu$m). This peak is due to the highly nonuniform oxidation rate in that region. As time progresses, the peak shifts to the left, further into the nitride mask, and gives rise to a late peak. As expected, stress decreases as the viscosity gets lower.

In the second part, we repeat the same simulations with the silicon nitride layer modeled as an elastic material. The Young's modulus and the Poisson's ratio of silicon nitride are assumed to be 3.29×10^{11} dynes·cm^{-2} and 0.266 respectively [6]. The thickness of the nitride layer is 0.1μm. The final shapes of the oxide and the nitride layer are shown in Fig. 3a, 3b, and 3c. As we can see, the nitride layer bends less as the oxide becomes less viscous and flows more readily. The corresponding values for peak stress are 2×10^{11}, 1.4×10^{11}, and 4.6×10^{10} dynes·cm^{-2} respectively. The first two values are unrealistically high because they are the same order of magnitude as the elastic moduli of oxide. We find that in general we need those stress values in order to bend the nitride mask to a degree comparable to what is found in experiments. To keep stress down to a realistic level, silicon nitride must deform elastoplastically or viscoelastically. Unfortunately we don't have data on those behaviors.

4 Summary

A boundary element technique has been developed to model thermal oxidation of silicon in two dimensions. It can handle a wide range of relaxtion times for the viscoelastic flow of oxide. Simulations of some simple structures have been demonstrated. Preliminary results indicate that it is inadequate to treat silicon nitride as an elastic material. A comprehensive characterization of silicon nitride is clearly needed.

5 Acknowledgment

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Appendix

The fundamental solutions for viscoelastic flow induced by constant-velocity loading are given below. Note that the subscripts of ϕ denote partial derivatives.

$$
\begin{aligned}
\sigma^*_{111} &= [-K_\alpha(2y\phi_{zy} + 3\phi_z) - K_\beta(y\phi_{zy} + 5\phi_z)]E \\
\sigma^*_{121} &= [K_\alpha(2y\phi_{zz} - \phi_y) + K_\beta(y\phi_{zz} - 4\phi_y)]E \\
\sigma^*_{221} &= [K_\alpha(2y\phi_{zy} - \phi_z) + K_\beta(y\phi_{zy} + 3\phi_z)]E \\
u^*_{11} &= -7K_\alpha(1-2\nu)y\phi_y - (y\phi_y + \phi)\Delta t \\
u^*_{21} &= 7K_\alpha(1-2\nu)y\phi_z + y\phi_z\Delta t
\end{aligned}
$$

$$
\begin{aligned}
\sigma^*_{112} &= [K_\alpha(2y\phi_{zz} - 3\phi_y) + K_\beta(y\phi_{zz} + 2\phi_y)]E \\
\sigma^*_{122} &= [K_\alpha(2y\phi_{zy} + \phi_z) + K_\beta(y\phi_{zy} - 3\phi_z)]E \\
\sigma^*_{222} &= [K_\alpha(2y\phi_{zz} + \phi_y) + K_\beta(y\phi_{zz} + 4\phi_y)]E \\
u^*_{12} &= 7K_\alpha(1-2\nu)y\phi_z + y\phi_z\Delta t \\
u^*_{22} &= 7K_\alpha(1-2\nu)y\phi_y + (y\phi_y - \phi)\Delta t
\end{aligned}
$$

and

$$
\begin{aligned}
\phi(\vec{r}) &= \frac{1}{2}\log[2(\cosh(y) - \sin(x))] \\
K_\alpha &= \frac{6}{7}\frac{\eta}{E}[1 - \exp(-\frac{\Delta t}{\tau_\alpha})] \\
K_\beta &= \frac{2}{7}\frac{\eta}{E}[1 - \exp(-\frac{\Delta t}{\tau_\beta})] \\
\tau_\alpha &= \frac{3(3-4\nu)\eta}{E} \\
\tau_\beta &= \frac{2(1+v)\eta}{E} \\
&= \frac{\eta}{G}
\end{aligned}
$$

where E is the Young's modulus, G the shear modulus, and ν the Poisson's ratio. The fundamental solutions are functions of time; they are evaluated at the end of a time step of size Δt. K_α and K_β decay exponentially with a time constant of τ_α and τ_β respectively when the load is removed.

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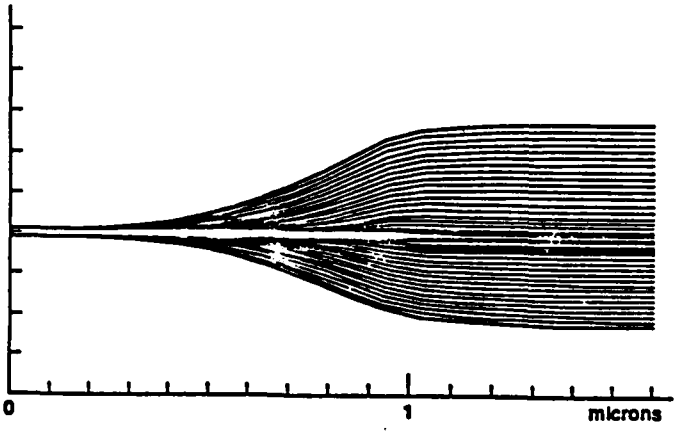
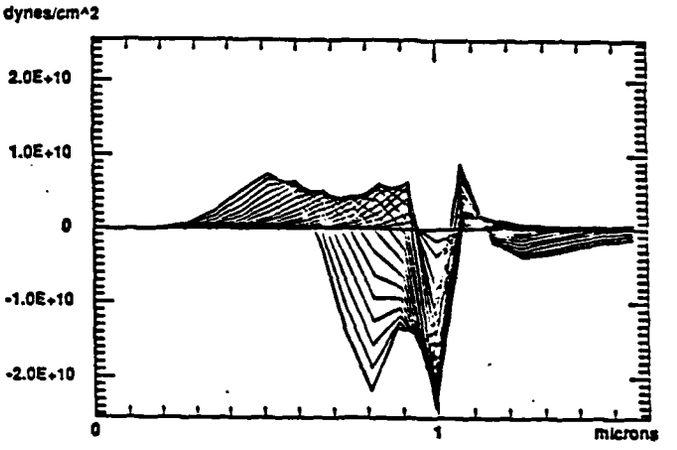
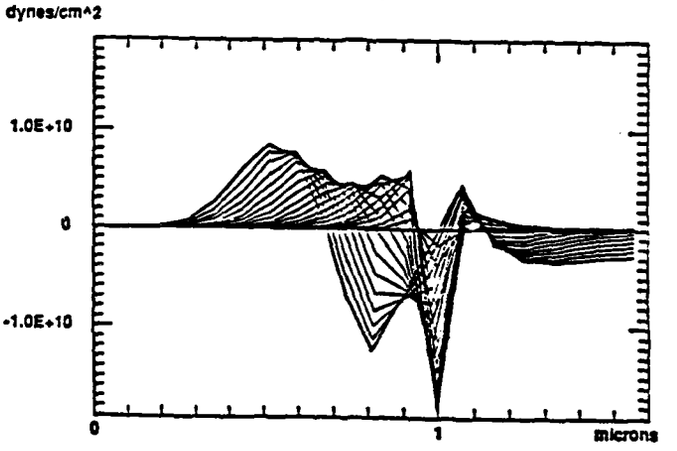


Fig. 1. Outline of oxide for every time step. Final field oxide thickness is 0.5μm.



(2a)



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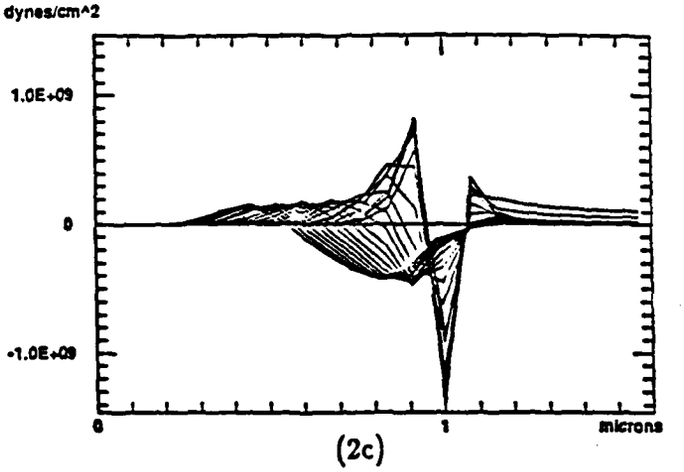
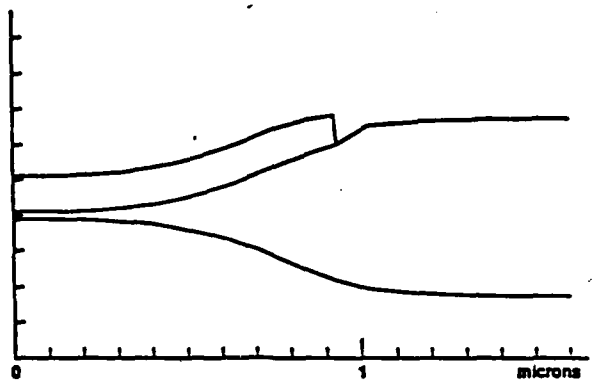
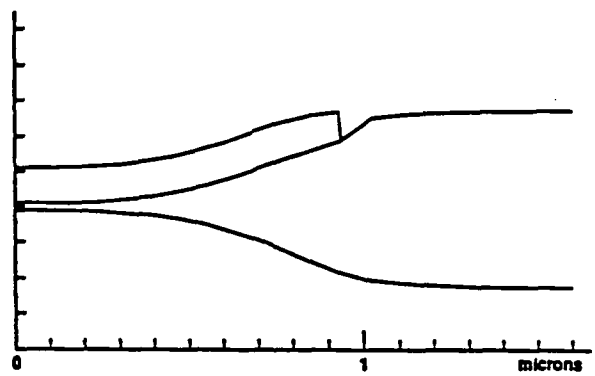


(2c)

Fig 2. Normal surface traction at the oxide-interface. (a) $\tau_\beta = 100$ hours, (b) 1 hour, (c) 1 miniute.



(a)



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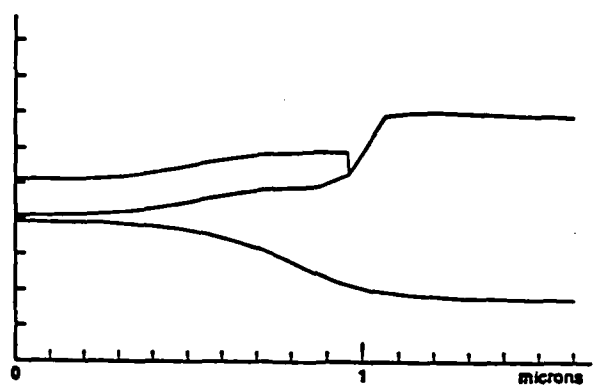

(c)

Fig 3. Effect of 0.1μm silicon nitride on oxide shape. (a) $\tau_\beta = 100$ hours, (b) 1 hour, (c) 1 miniute.

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