Derived Boundary Conditions for Viscous Thermal Oxidation Equations in Pressure Potential Form

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Abstract

Boundary conditions for viscous flow thermal oxidation equations in pressure potential form are derived in a way which is physically consistent and also convenient for practical implementation. A role of the incompressibility constraint on oxide boundary is emphasised. A possibility to employ the standard piecewise linear finite element or finite volume discretization schemes is justified. Importance and correctness of the derived boundary conditions are practically demonstrated in the simulation of the standard LOCOS process.

1. Introduction

The incompressible viscous flow equations are commonly employed for the modeling of thermal oxidation processes at high temperatures. However, numerical treatment of the incompressibility constraint typically requires special concerns with the selection of discrete approximation spaces and solving procedures [1]. An effective alternative is to employ the pressure potential form (PPF) of the viscous flow equations [2]. For an oxide region Ω with boundary Γ (Fig. 1), it is defined by:

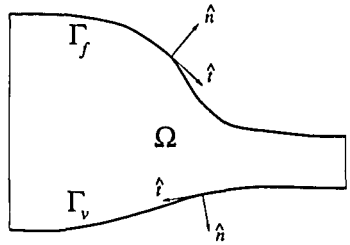

Figure 1: Oxide region and interfaces.

$$-\mu\nabla^2\vec{v} + \nabla p = 0 \quad \text{in } \Omega \qquad (1)$$

$$\nabla^2 p = 0 \quad \text{in } \Omega \qquad (2)$$

$$\nabla \cdot \vec{v} = 0 \quad \text{on } \Gamma \qquad (3)$$

where $\vec{v}$ is oxide velocity, p is mean pressure and μ is dynamic oxide viscosity. It should be emphasised that the boundary constraint (3) is the necessary "boundary" condition for the equivalence of PPF and the original Stoke's problem [2].

The two essential boundary conditions (BCs) for thermal oxidation equations are: $\vec{v} \cdot \hat{n} = -V$ on the Si-SiO_2 interface (Γ_v) where V is the Deal-Grove oxide velocity, and $\sigma \cdot \hat{n} = \vec{T}$ on the force balance interface (Γ_f), where σ and $\vec{T}$ are the total stress

tensor and a surface force vector. Here $\hat{n}$ is an outward unit normal vector on the boundary Γ. It is used with the corresponding unit tangential vector $\hat{t}$ (Fig. 1) to erect a local boundary coordinate system $(\hat{t},\hat{n})$.

An important advantage of PPF is a simple and straightforward formulation of the weak statements for (1) and (2) as:

$$\int_{\Omega} \mu \nabla v_i \cdot \nabla \phi + \int_{\Omega} \frac{\partial p}{\partial x_i}\phi - \int_{\Gamma_f} \mu \frac{\partial v_i}{\partial n}\phi = 0 \tag{4}$$

$$\int_{\Omega} \nabla p \cdot \nabla \phi - \int_{\Gamma_v} \frac{\partial p}{\partial n}\phi = 0. \tag{5}$$

However, notice that a practical implementation of (4) and (5) requires the specification of additional Neumann BCs; for pressure on Γ_v and velocity components on Γ_f. This paper is intended to demonstrate a possible circumvention of that problem.

2. Pressure Neumann BC on the *Si–SiO*$_2$ Interface (Γ_v)

The ambiguity in the pressure Neumann BC formulation is today completely resolved identifying it simply with the normal component of the momentum equation (1) on Γ_v [2]. However, since second derivatives appear in this formulation, its practical implementation in (5) is not straightforward.

We have considered here as more convenient to derived the pressure Neumann BC directly within the weighted residual form. Multiplying momentum equation (1) by $\nabla\phi$ and using identity $-\nabla^2\vec{v} = \nabla \times (\nabla \times \vec{v})$ that holds for $\nabla \cdot \vec{v} = 0$ we have

$$\int_{\Omega} \nabla p \cdot \nabla \phi = \int_{\Omega} \mu [\nabla \times (\nabla \times \vec{v})] \cdot \nabla \phi. \tag{6}$$

Integrating by parts in the right hand side of (6) we obtain

$$\int_{\Omega} \nabla p \cdot \nabla \phi - \int_{\Gamma_v} \mu \vec{g} \cdot \nabla \phi = 0 \quad \text{where} \quad \vec{g} = (\hat{n} \cdot \nabla)\vec{v} - \nabla(\vec{v} \cdot \hat{n}). \tag{7}$$

Notice that (7) actually represents the weak residual statement (5) with incorporated pressure Neumann BC. The integral term on Γ_v involves a vector-valued function $\vec{g}$ that verifies $\vec{g} \cdot \hat{n} = 0$ and also allows implementation of the conventional piecewise-linear approximation functions.

3. Velocity Neumann BC on the Force Balance Interface (Γ_f)

The only physically relevant basis for the formulation of the Neumann BCs for velocity components on Γ_f are: (i) the balance of the tangential force components, and (ii) the boundary constraint (3). Notice that the balance of the normal force components is not appropriate here since it already serves as the essential pressure BC on Γ_f.

For simplicity, we consider here only a 2D case with traction free interface Γ_f. In the local boundary coordinates with velocity components (v_t,v_n), the balance of tangential forces and the divergence free condition can be expressed as:

$$\frac{\partial v_n}{\partial t} + \frac{\partial v_t}{\partial n} = 0 \quad \text{and} \quad \frac{\partial v_n}{\partial n} + \frac{\partial v_t}{\partial t} = 0. \tag{8}$$

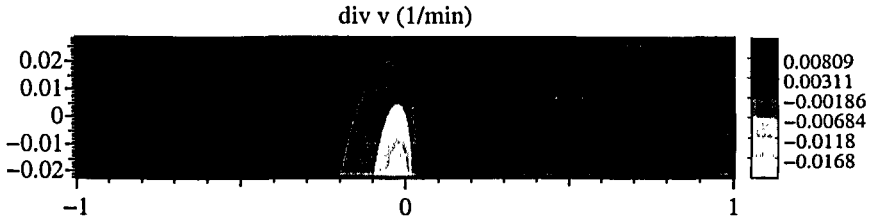

Figure 2: Velocity divergence obtained with the homogenous Neumann pressure BC in an initial pad oxide.

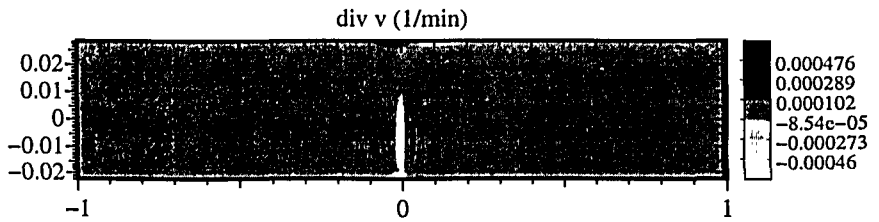

Figure 3: Velocity divergence obtained with the derived pressure BC in an initial pad oxide.

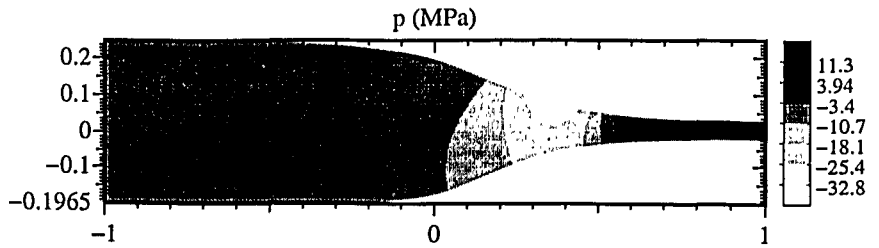

Figure 4: Pressure distribution obtained with the homogenous Neumann pressure BC at the end of LOCOS formation.

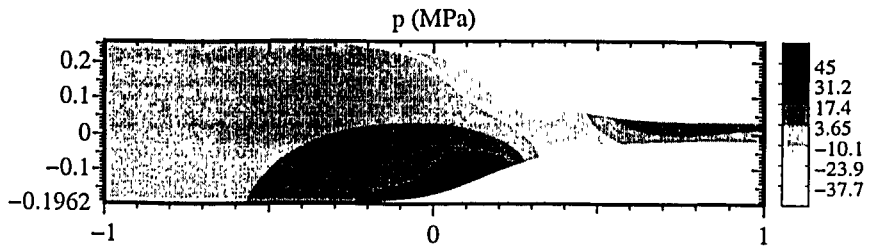

Figure 5: Pressure distribution obtained with the derived pressure BC at the end of LOCOS formation.

Introducing global velocity components (v_x,v_y) in (8) using $v_n = v_x n_x + v_y n_y$ and $v_t = v_x t_x + v_y t_y$, we obtain a system:

$$\begin{pmatrix} n_x & n_y \\ t_x & t_y \end{pmatrix} \cdot \begin{pmatrix} \frac{\partial v_x}{\partial n} \\ \frac{\partial v_y}{\partial n} \end{pmatrix} = - \begin{pmatrix} t_x & t_y \\ n_x & n_y \end{pmatrix} \cdot \begin{pmatrix} \frac{\partial v_x}{\partial t} \\ \frac{\partial v_y}{\partial t} \end{pmatrix}. \tag{9}$$

The solution of (9) gives the unique set of Neumann BCs for velocity components:

$$\frac{\partial v_x}{\partial n} = (-n_x n_y + t_x t_y) \frac{\partial v_x}{\partial t} + \left(-n_y^2 + t_y^2\right) \frac{\partial v_y}{\partial t} \tag{10}$$

$$\frac{\partial v_y}{\partial n} = \left(n_x^2 - t_x^2\right) \frac{\partial v_x}{\partial t} + (n_x n_y - t_x t_y) \frac{\partial v_y}{\partial t} \tag{11}$$

which are defined in terms of the first order tangential derivatives of the global velocity components on Γ_f.

4. Case Study

It should be emphasised that some of the fractional step pressure correction methods based on PPF still relay on the simple homogeneous Neumann BC for pressure [3]. In order to demonstrate the importance of using the physically consistent derived BCs for viscous thermal oxidation equations in PPF, we consider here some simulation results of the standard LOCOS process.

Fig. 2 shows that the usage of the inconsistent homogenous Neumann BC for pressure results in significant non-physical compressibility of the pad oxide body. On the other side, it is not the case with the application of the derived inhomogeneous pressure BC, as it is shown in Fig. 3. Additionally, Figs. 4 and 5 show significantly different distributions of the pressure in the final LOCOS structure when the homogenous and correct inhomogeneous derived Neumann BC are used.

5. Conclusion

The advantage of viscous thermal oxidation equations in PPF is the application of equal-order interpolation for velocity and pressure in standard finite element or finite volume discretization methods. The required additional boundary conditions are derived by appropriate extensions of the governing viscous flow equations to the boundary. To this end, the momentum equation is employed to directly derive a weak pressure potential residual statement with incorporated Neumann pressure BC, while the incompressibility constraint on the boundary play an essential role in derivation of the Neumann BCs for velocity components.

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