Construction of an electromagnetic – TCAD transient solver: Interface & boundary condition subtleties

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October 10, 2009
Overview

- Introduction
- Transient Electromagnetic-TCAD
- Interface conditions
- Boundary conditions
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Introduction

Aim of the work:

- Support to circuit model development of devices by applying first-principle evaluation of electromagnetic responses
- Replacement of circuit models by full-wave characterizations
- Allowance of these approaches directly in the time regime

This requires two developments:

- Construction of a transient field solver for semiconductors and large-signal electromagnetic fields
- Construction of a circuit-field co-simulation framework
Transient Electromagnetic-TCAD

The transient electromagnetic-TCAD equations are:

**Maxwell equations**

\[ \nabla \cdot \mathbf{D} = \rho \]
\[ \nabla \cdot \mathbf{B} = 0 \]
\[ \nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \]
\[ \nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \]

**Conductors**

\[ \nabla \cdot \mathbf{J} = -j\omega \rho \]
\[ \mathbf{J} = \sigma \mathbf{E} \]

**Semi-conductors**

\[ \nabla \cdot \mathbf{J}_n - qj\omega n = U(n, p) \]
\[ \nabla \cdot \mathbf{J}_p + qj\omega p = -U(n, p) \]
\[ \rho = q(p - n + N_D - N_A) \]
\[ \mathbf{J}_n = q\mu_n n \mathbf{E} + kT\mu_n \nabla n \]
\[ \mathbf{J}_n = q\mu_p p \mathbf{E} - kT\mu_p \nabla p \]
\[ \mathbf{J} = \mathbf{J}_n + \mathbf{J}_p \]

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Transient Electromagnetic-TCAD

- TCAD solves for
  - Voltages $V$, and carrier densities $n$, $p$ or $V$, $\phi_p$, $\phi_n$ but NOT $E$
- Set up the Maxwell equations in potential formulation $V$, $A$

**Gauss**

$- \nabla \cdot (\varepsilon \nabla V + \frac{\partial A}{\partial t}) = \rho(V,A)$

**Maxwell-Ampere**

$\nabla \times \nabla \times A = \mu J(V,A) - \mu \varepsilon \frac{\partial}{\partial t}(\nabla V + \frac{\partial A}{\partial t})$

**Gauge condition**

$\nabla \cdot A + \frac{\xi}{c^2} \frac{\partial V}{\partial t} = 0\ ,\ \xi = 1$ Lorentz

$E = -\nabla V - \frac{\partial A}{\partial t}$  
$B = \nabla \times A$

$D = \varepsilon E$  
$B = \mu H$

System to be solved
TCAD experience

- Use Gauss’ law to compute $V$
- In insulators Gauss’ law is used to compute $V$

- Use the current-continuity equations to compute $\phi_p, \phi_n$
- Metals are usually ‘ignored’ (i.e. replaced by ideal boundary conditions)

- For skin effects, induced substrate currents this is not permissible.
- We must now treat metals using Ohm’s law: this gives (again) an equation for $V$
Interfaces: metal/insulator

- What to do at metal/insulator interface points?
- Should we use Gauss’ law or/and Ohm’s law?

- At metal/insulator interface points, there is current present
- use Ohm’s law to compute $V$
- Next, Gauss’ law is used for computing the surface charge at these nodes.
Interfaces: metal/semiconductor

- The metal/semiconductor interface nodes also carry current
- **use Ohm’s law to compute V**
- However, doping generates a build-in potential
- Fixed voltage jump, when passing through an M/S interface
- Consider a donut of a diode and metal

![Diagram of a donut with P-type and N-type regions](image)

- X1
- X2
- X3
- Metal
- V
- P-type
- N-type

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Interfaces: metal/semiconductor

- \( V_{\text{semi}} = V_{\text{metal}} - \delta V \)

- \( \phi_p = \phi_n = V_{\text{metal}} \)

- For the carrier concentrations we assume infinitely large recombination velocities

- \( p-n+N_D = 0 \) and \( pn = n_i^2 \)

- This allows us to obtain \( \delta V \) from the doping

- Only one variable (V) is computed at M/S interfaces!
Triple points: metal/semiconductor/insulator

- Take half-sized jumps @ triple points (lines)
- The voltage plots can give ‘counter-intuitive’ results due to penetration of the build-in potential into insulators
Boundary conditions

- Internal boundary conditions
  - These are boundary conditions mimicking actual measurements set ups.

- External boundary conditions
  - These are the boundary conditions for the surface of the simulation domain
  - Beware that there are **four** or **six** fields to be computed!

\[ V, A_x, A_y, A_z \text{ and possibly } \phi_p, \phi_n \]
Boundary conditions: Dirichlet

- Let us start simple: for a contact surface: \( V = V_{\text{ext}} \)
- This is a Dirichlet’ boundary condition
- From TCAD, we borrow the idea that \( E_n = E \cdot n = 0 \) for non-contact boundary points

Pure TCAD: \( E = -\nabla V \Rightarrow E_n = -\frac{\partial V}{\partial n} = 0 \)

EM TCAD: \( E = -\nabla V - \frac{\partial A}{\partial t} \Rightarrow E_n = -\frac{\partial V}{\partial n} - \frac{\partial}{\partial t} (A \cdot n) = 0 \)
Boundary conditions: Dirichlet

- We can extend the Dirichlet boundary conditions by taking \( A \cdot t = 0 \).
- Since \( \mathbf{B} = \text{curl} \, \mathbf{A} \) we have that \( \mathbf{B} \) is tangential to the surface.
Boundary conditions: Dirichlet

- Do not forget the gauge condition!

- Simultaneous obeying Dirichlet’s boundary conditions for $A$ and the gauge condition requires that $A.n|_{in}$ and $A.n|_{out}$ and $dV/dt$ are related.

- The gauge condition is void for these boundary conditions, since its evaluation requires the variable $A.n$ from the outside which is not part of the set of degrees of freedom.

- As a consequence, for links bouncing on the surface of the simulation domain, the gauge condition should not be inserted for lifting the singular character of $\nabla \times \nabla \times A$. 
Boundary conditions: Neumann

- We can start from Neumann boundary conditions for $\mathbf{A}$.
- $90^\circ$ Mur boundary conditions for potentials is implemented.
Boundary conditions: Neumann

- Missing ‘\(B\)’ can be assigned to \(\frac{\partial A_\parallel}{\partial n}\)

\[
\frac{\partial A_\parallel}{\partial n}
\]
Boundary conditions: Neumann

\[ \frac{\partial A_{\parallel}}{\partial n} \]

can be assigned to radiation of TE wave

\[ \frac{\partial A_{\parallel}}{\partial n} - j\omega \frac{A_{\parallel}}{c} = 0 \]
# Boundary conditions overview

<table>
<thead>
<tr>
<th>Default EM-TCAD</th>
<th>Radiative</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V$ : Dirichlet at contact</td>
<td>$V$ : Dirichlet at contact</td>
</tr>
<tr>
<td>$V$ : Neumann at non-contact</td>
<td>$V$ : Dirichlet at non-contact (e.g. $V=0$)</td>
</tr>
<tr>
<td>$A_{\parallel}$ : Dirichlet</td>
<td>$A_{\parallel}$ : Neumann</td>
</tr>
<tr>
<td>$A_{\perp}$ : match of gauge condition</td>
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Conclusions

- Interface conditions are non-trivial for EM+TCAD

- Boundary conditions require a careful analysis concerning
  - Desired character of the boundary condition
  - Discretization scheme
  - Respecting the gauge condition