ICESTARS

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

WP3 – Wim Schoenmaker/MAGWEL

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Overview

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

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:

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

Maxwell equations

Conductors

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

Semi-conductors

$$\nabla \cdot \mathbf{J}_n - q\, j\omega\, n = U(n,p)$$
$$\nabla \cdot \mathbf{J}_p + q\, j\omega\, p = -U(n,p)$$

$$\rho = q(p - n + N_D - N_A)$$
$$\mathbf{J}_n = q\mu_n n\mathbf{E} + kT\mu_n \nabla n$$
$$\mathbf{J}_n = q\mu_p p\mathbf{E} - kT\mu_p \nabla p$$
$$\mathbf{J} = \mathbf{J}_n + \mathbf{J}_p$$

Drift (EM)

Diffusion (TCAD)

Transient Electromagnetic-TCAD

- TCAD solves for
  - Voltages V, and carrier densities n, p or V , ϕ_p , ϕ_n but NOT ***E***
- Set up the Maxwell equations in potential formulation V, ***A***

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

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

Gauge condition → $$\nabla \cdot \mathbf{A} + \frac{\xi}{c^2}\frac{\partial V}{\partial t} = 0 \quad , \quad \xi = 1 \text{ Lorentz}$$

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

$$\mathbf{B} = \nabla \times \mathbf{A}$$

$$\mathbf{D} = \varepsilon \mathbf{E}$$

$$\mathbf{B} = \mu \mathbf{H}$$

System to be solved

TCAD experience

- Use Gauss' law to compute V
- In insulators Gauss' law is used to compute V

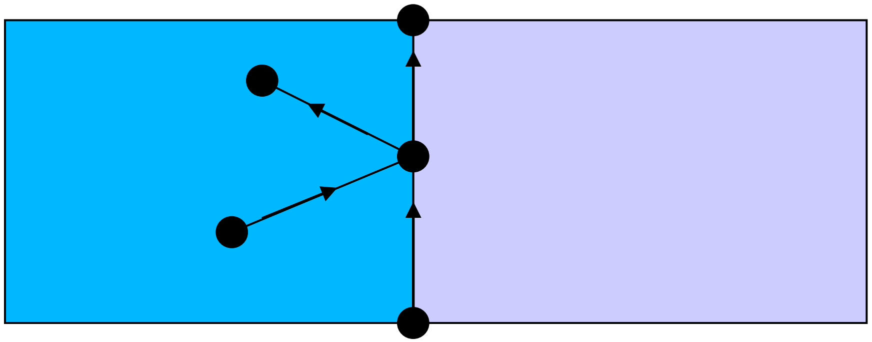
- Use the current-continuity equations to compute ϕ_p , ϕ_n
- Metals are usually 'ignored' (i.e. replaced by ideal boundary conditions

- 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

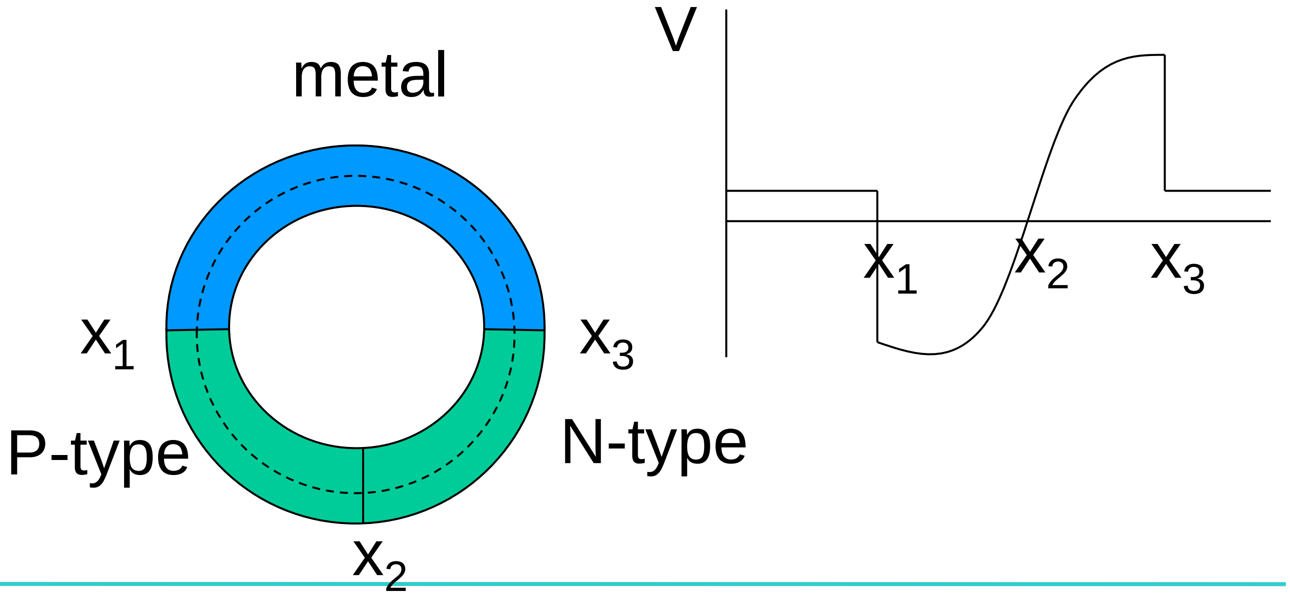
- What to do at metal/insulator interface points?
- Should we use Gauss' law or/and Ohm's law?

- 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



Interfaces: metal/semiconductor

- $V_{semi} = V_{metal} - \delta V$

- $\phi_p = \phi_n = V_{metal}$

- For the carrier concentrations we assume infinitely large recombination velocities

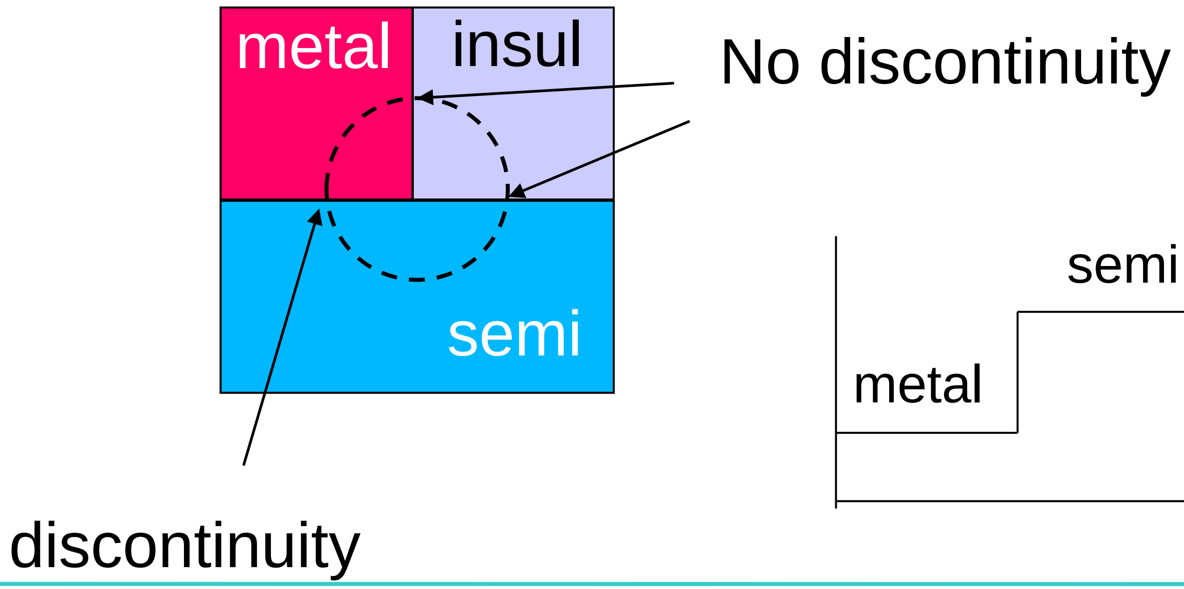
- $p\text{-}n+N_D = 0$ and $pn = n_i^2$

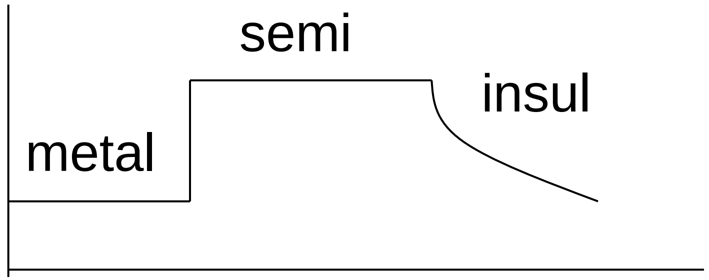
- This allows us to obtain δV from the doping

- **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!

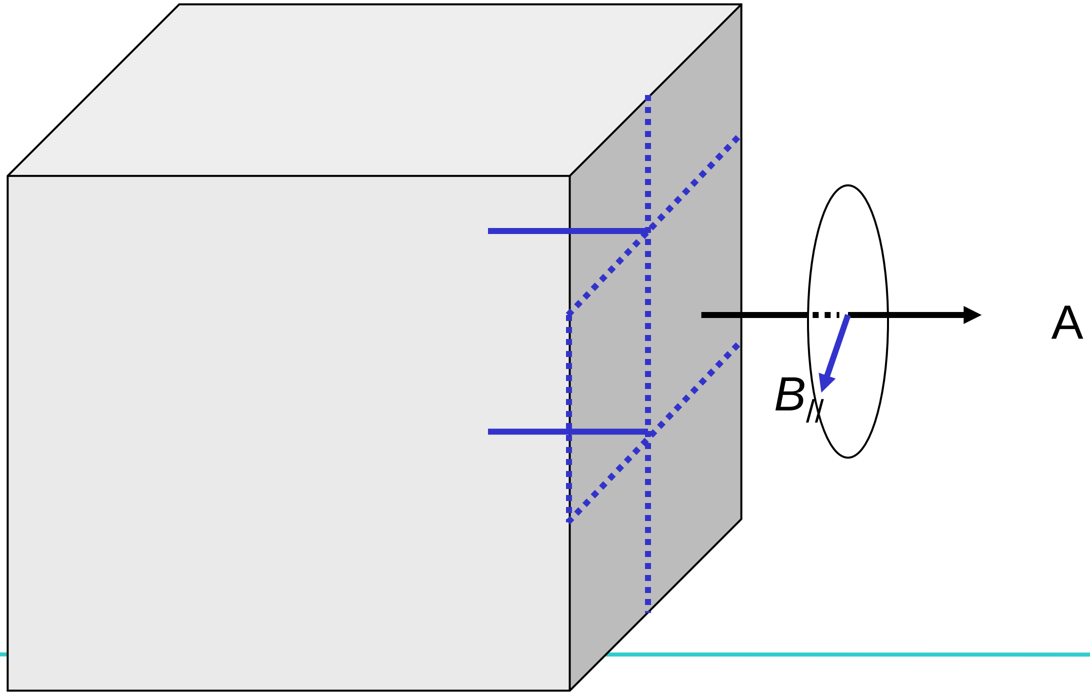
$$V\ ,\ A_x\ ,\ A_y\ ,\ A_z \text{ and possibly } \phi_p\ ,\ \phi_n$$

Boundary conditions: Dirichlet

- *Let us start simple:* for a contact surface: $V=V_{ext}$
- This is a Dirichlet' boundary condition
- From TCAD, we borrow the idea that E_n = ***E.n*** =0 for non-contact boundary points
- Pure TCAD: $$\mathbf{E} = -\nabla V \Rightarrow E_n = -\frac{\partial V}{\partial \mathbf{n}} = 0$$
- EM TCAD : $$\mathbf{E} = -\nabla V - \frac{\partial \mathbf{A}}{\partial t} \Rightarrow E_n = -\frac{\partial V}{\partial \mathbf{n}} - \frac{\partial}{\partial t}(\mathbf{A}\cdot\mathbf{n}) = 0$$

Boundary conditions: Dirichlet

- We can extend the Dirichlet boundary conditions by taking $\boldsymbol{A}.\boldsymbol{t} = 0$
- Since ***B***=curl ***A*** we have that **B** is tangential to the surface



Boundary conditions: Dirichlet

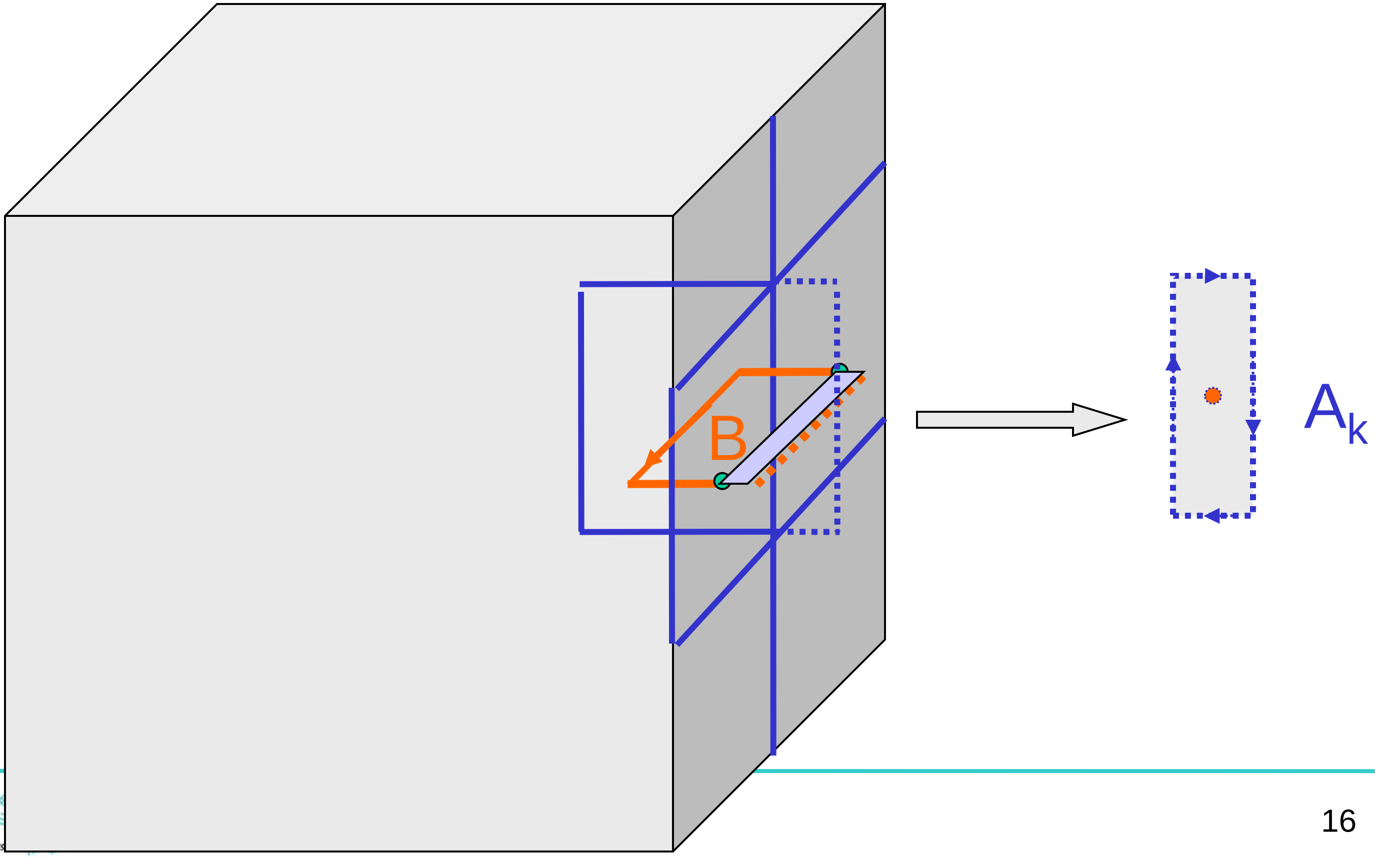
- Do not forget the gauge condition!
- Simultaneous obeying Dirichlet's boundary conditions for A and the gauge condition requires that $\boldsymbol{A.n}|_{in}$ ***and*** $\boldsymbol{A.n}|_{out}$ and dV/dt are related
- **The gauge condition is void for these boundary condition, since its evaluation 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 $\nabla \times \nabla \times \mathbf{A}$

Boundary conditions: Neumann

- We can start from Neumann boundary conditions for **A**
- 90^0 Mur boundary conditions for potentials is implemented

Boundary conditions: Neumann

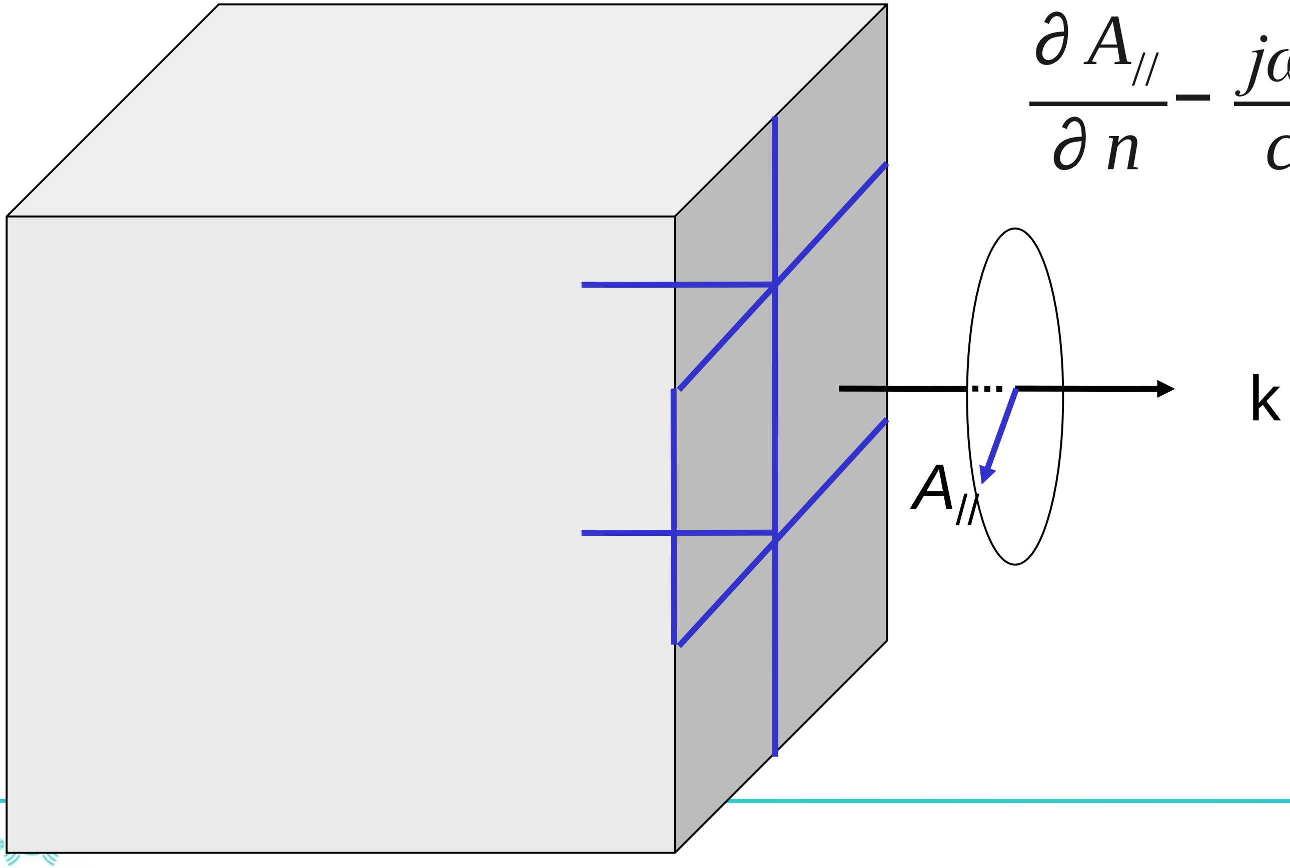
- Missing '**B**' can be assigned to $\dfrac{\partial A_{//}}{\partial n}$



Boundary conditions: Neumann

$\frac{\partial A_{//}}{\partial n}$ can be assigned to radiation of TE wave

$$\frac{\partial A_{//}}{\partial n} - \frac{j\omega}{c} A_{//} = 0$$



Boundary conditions overview

Default EM-TCAD	Radiative
V : Dirichlet at contact V : Neumann at non-contact	V : Dirichlet at contact V : Diriclet at non-contact (e.g. V=0)
$A_{//}$: Dirichlet	$A_{//}$: Neumann
$A_{\perp}$: match of gauge condition	$A_{\perp}$: match of gauge condition

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