Numerical Multiscale Modeling of the Metal-Insulator-Metal Structures

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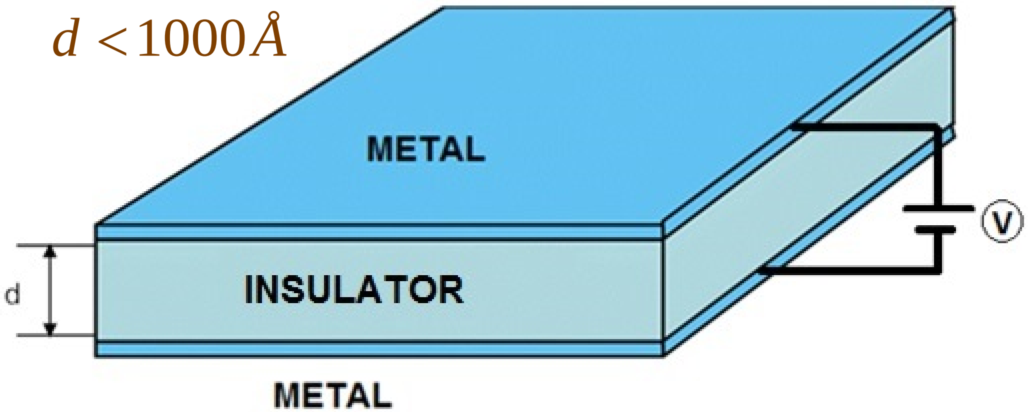
Introduction

$d < 1000\AA$



- Fowler-Nordheim cold emission

$$I = \int_S \mathbf{J} \cdot d\mathbf{A} = J_{med} A_S$$

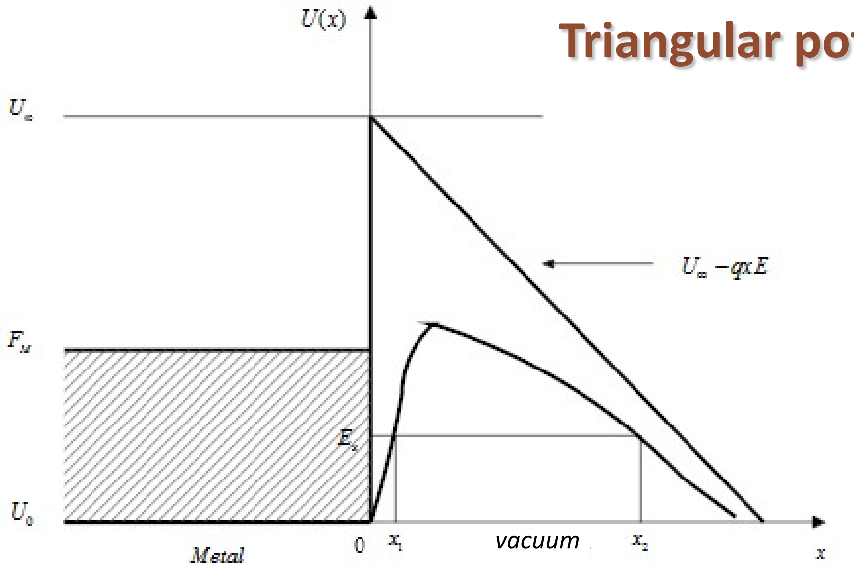
$$J = A \cdot E^2 \cdot Tr$$

$$A = \frac{q_0{}^3}{8\pi h\varphi}$$

$$Tr = \psi(x_2) \cdot \bar{\psi}(x_2)$$

“Simple solvable models of the tunneling barrier lead to equations … that get predictions of emission current density too low by a factor of 100 or more.” (Wikipedia, Field electron emission)

Introduction



Triangular potential barrier

$$U(x) = \begin{cases} 0, & x < 0 \\ U_\infty - q_0 E x, & x > 0 \end{cases}$$

without image force

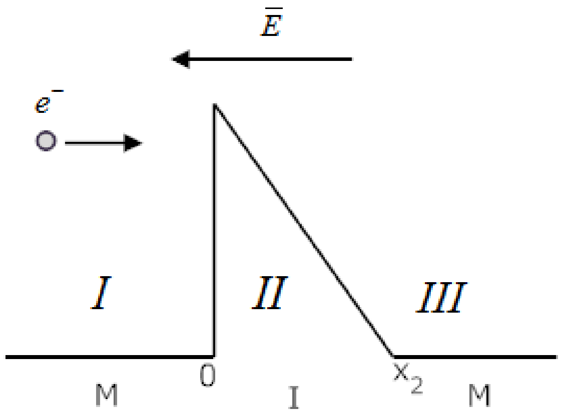
Rounded potential barrier

$$U(x) = \begin{cases} 0, & x < 0 \\ U_\infty - q_0 E x - \dfrac{q_0^2}{16\pi\varepsilon x}, & x > 0 \end{cases}$$

with image force (Schottky–Nordheim barrier)

Introduction

Wentzel-Kramers-Brillouin (WKB) approximation



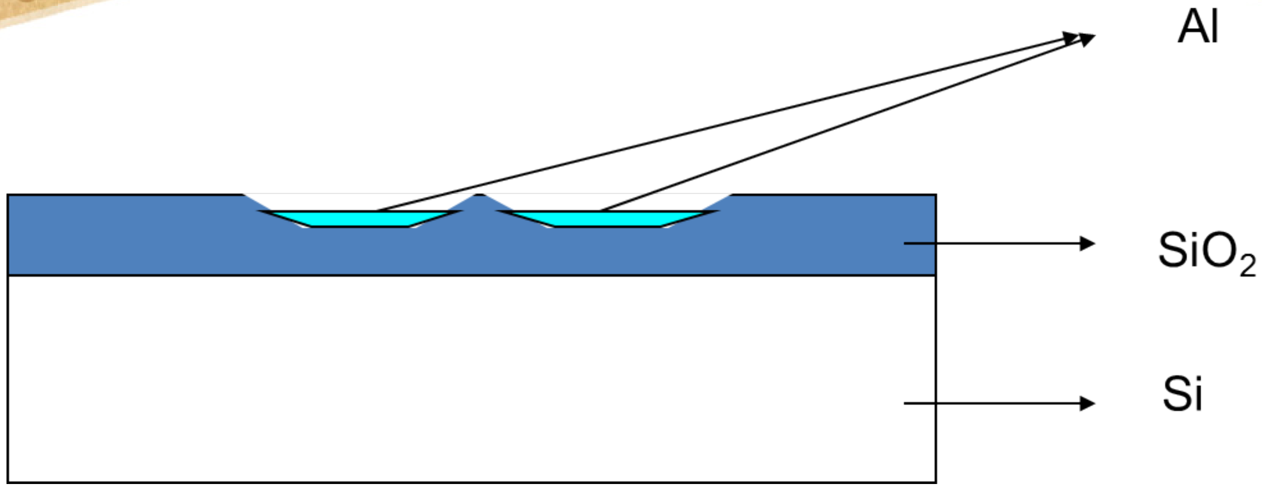
$$\psi''(x) + K(x)\psi(x) = 0$$

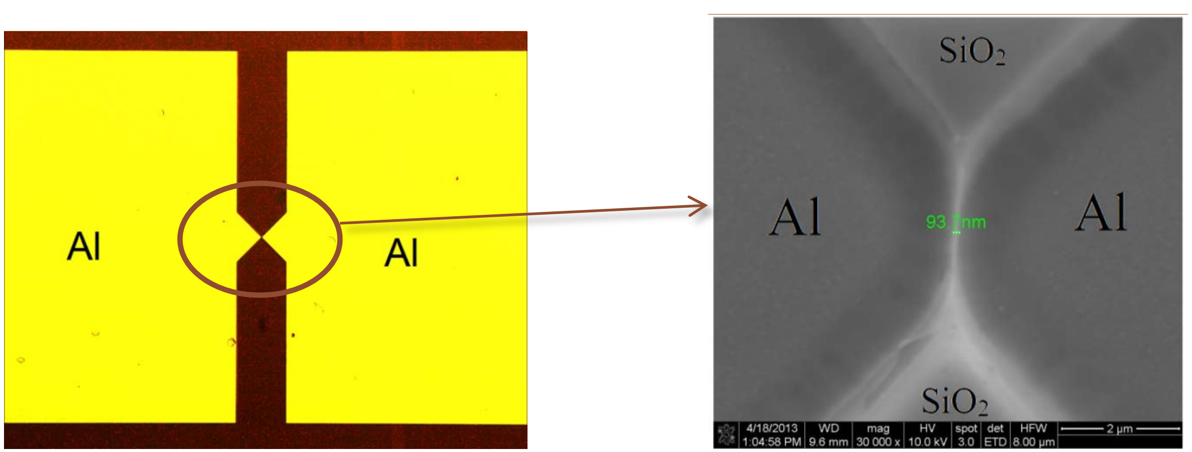
$$K(x) = \frac{2m}{\hbar^2}(w - U(x))$$

$$I, III: \quad \psi(x) = \frac{1}{[-K(x)]^{\frac{1}{4}}}\left\{C_1 \exp\left[\int \sqrt{-K(x)}dx\right] + C_2 \exp\left[-\int \sqrt{-K(x)}dx\right]\right\}$$

$$II: \quad \psi(x) = \frac{1}{[-K(x)]^{\frac{1}{4}}}\left\{C_1 \exp\left[\int \sqrt{K(x)}dx\right] + C_2 \exp\left[-\int \sqrt{K(x)}dx\right]\right\}$$

Electric field modeling in the test structure





Physical modeling:
- electrostatic field

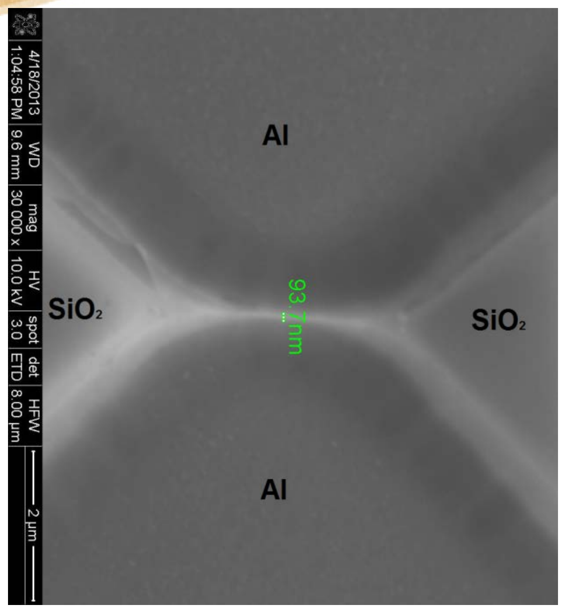
Geometric modeling:
- 2D top view
- 2D lateral view
- 3D

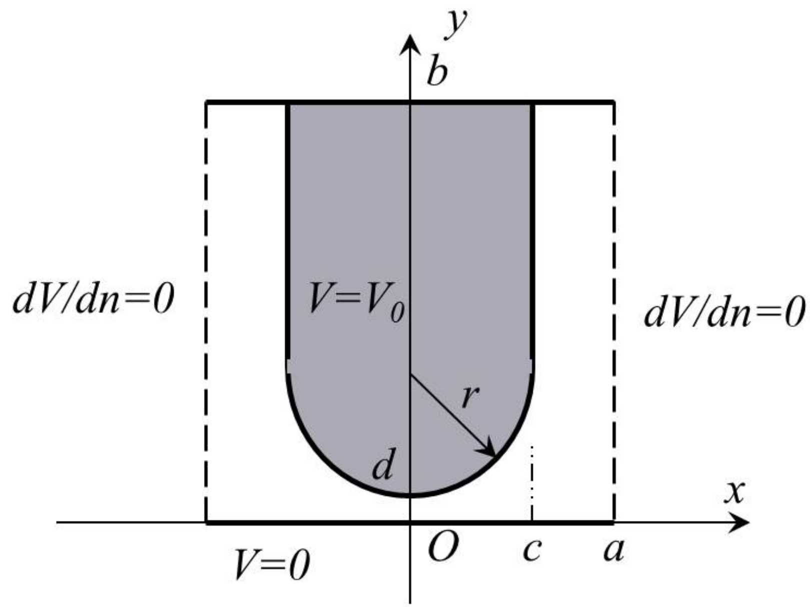
Methods:
- FEM
- Conformal mapping (edges)

Computation system:
- ATLAS Multiprocessor server from LMN/CIEAC/PUB

Electric field modeling in the test structure

❑ 2D top view :



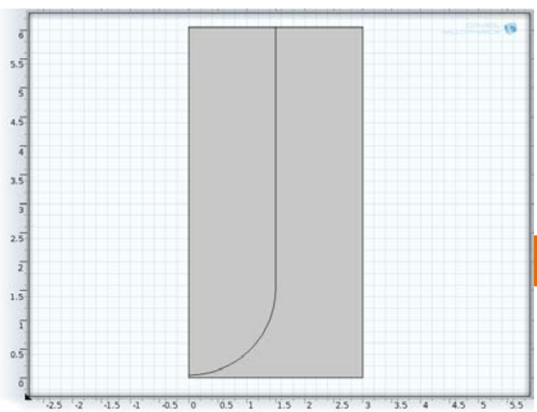


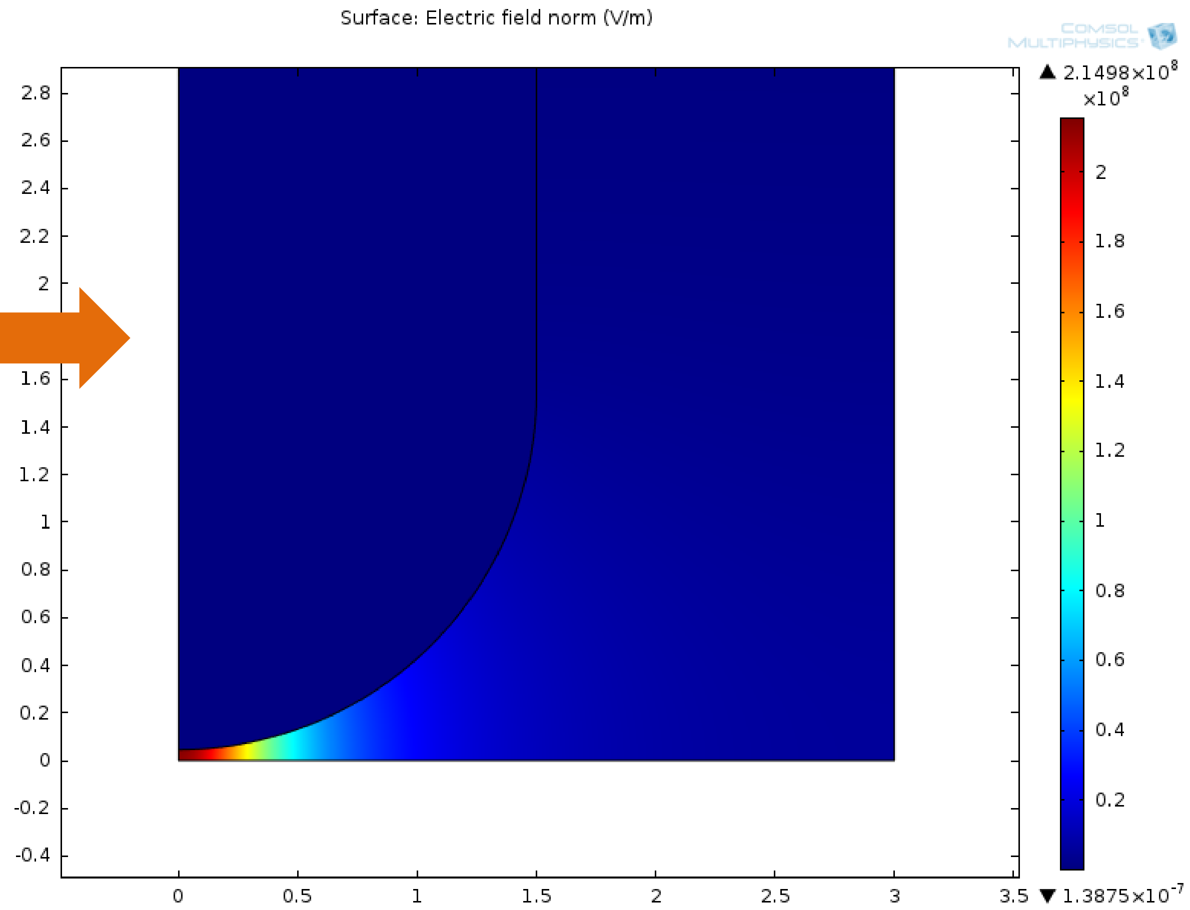
	Parameter	Value
1	d	47 nm
2	b	$4.5\mu m$
3	c	$1.5\mu m$
4	r	$1.5\mu m$
5	a	$3\mu m$
6	V_0	$10V$

Laplace equation was numerically solved for the scalar electrostatic potential V, considering mixed boundary conditions (Dirichlet and Neumann), using FEM.

Electric field modeling in the test structure

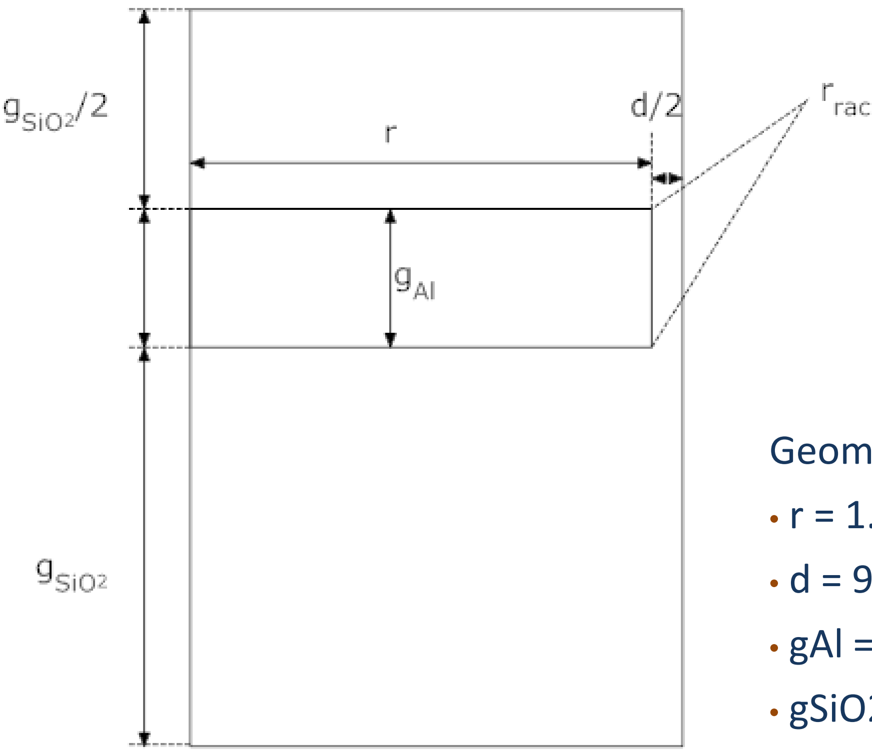
- **2D parallel-plane problem- top view**

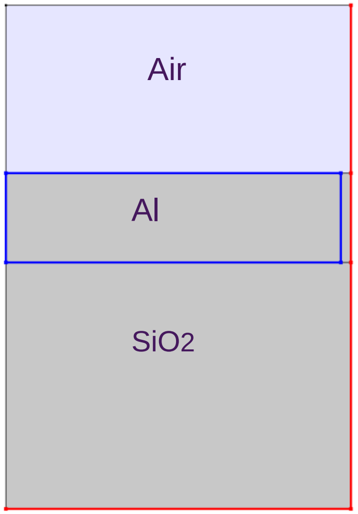




Electric field modeling in the test structure

❑ 2D parallel-plane problem- lateral view





Geometric parameters:

- r = 1.3 µm
- d = 93 nm
- gAl = 0.4 µm
- gSiO2 = 1.5 µm

- Electrostatic regime
- Boundary conditions:
  - with blue: V=10V
  - with red: V=0;
  - in rest: dV/dn=0

Purpose: study of sharp edge electrostatic effect (considering r_{rac} bending radius)

Electric field modeling in the test structure

❑ **Solution of the 2D parallel-plane problem- lateral view**

Electric field intensity (E) variation depending on the transition radius (r_{rac})

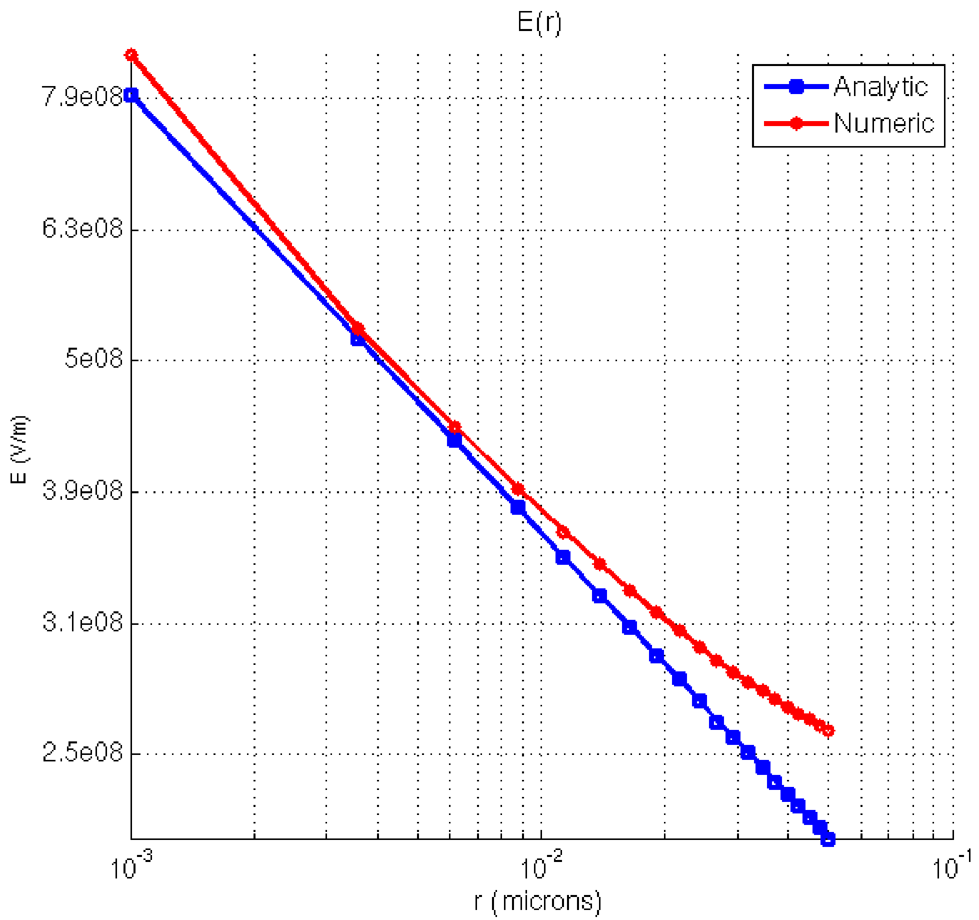
- **Numeric:** with FEM (COMSOL 4.4.)

  E_{max}= 1.034e9V/m

- **Analytic** (with conformal mapping):

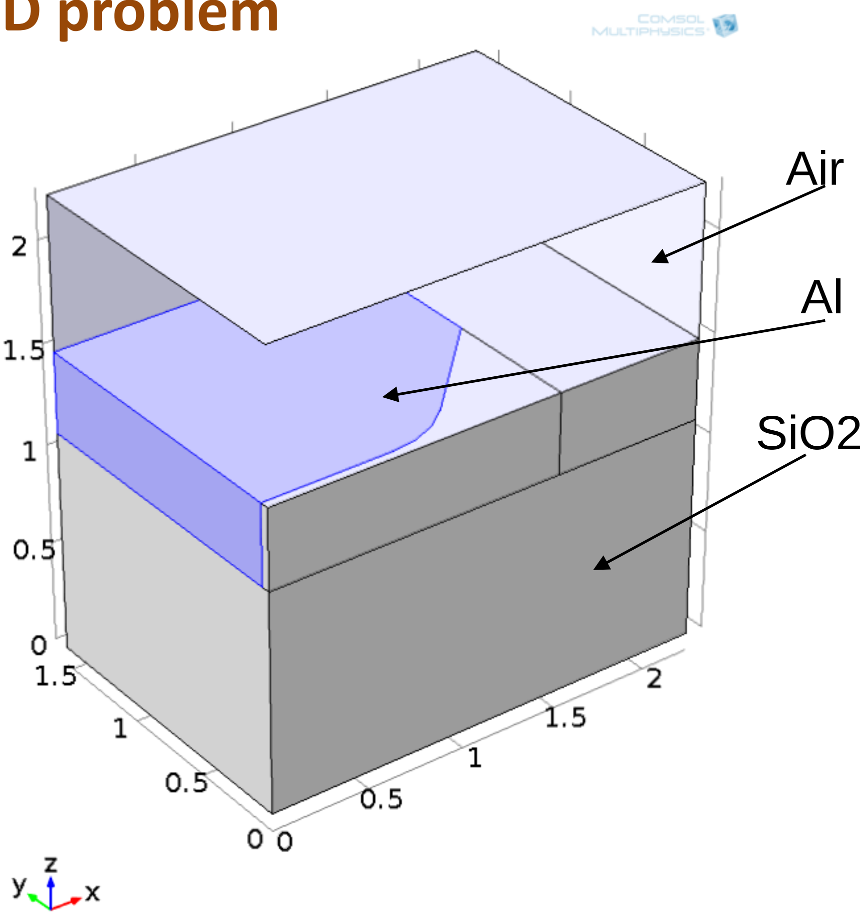
  E_{max}= 1.597e9V/m

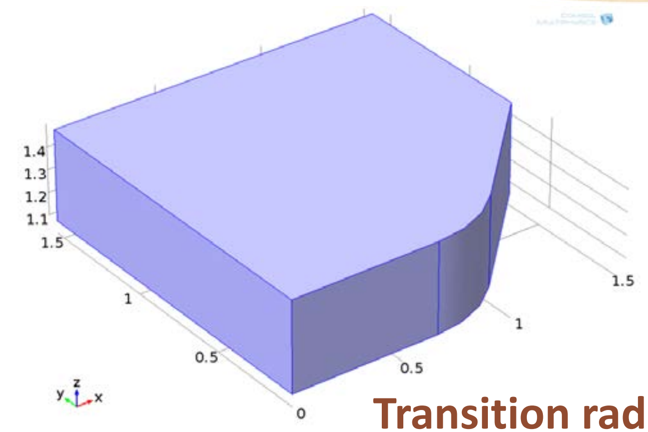
$$E/E_0 = 1.04 \cdot (r/d)^{-1/3}$$



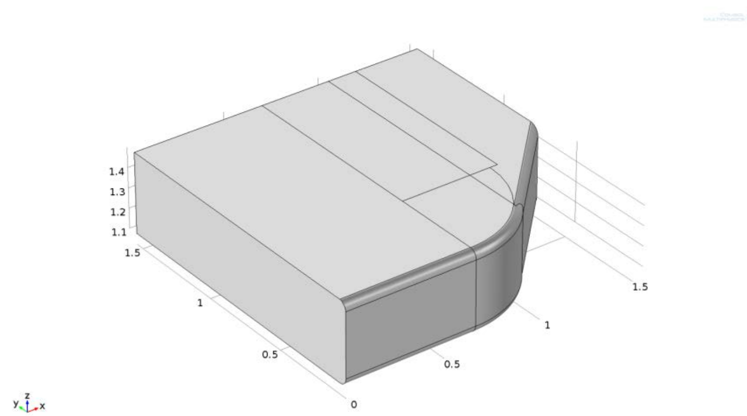
Electric field modeling in the test structure

- 3D problem





Transition radius 0



Transition radius 10 nm

Electric field modeling in the test structure

❑ 3D problem

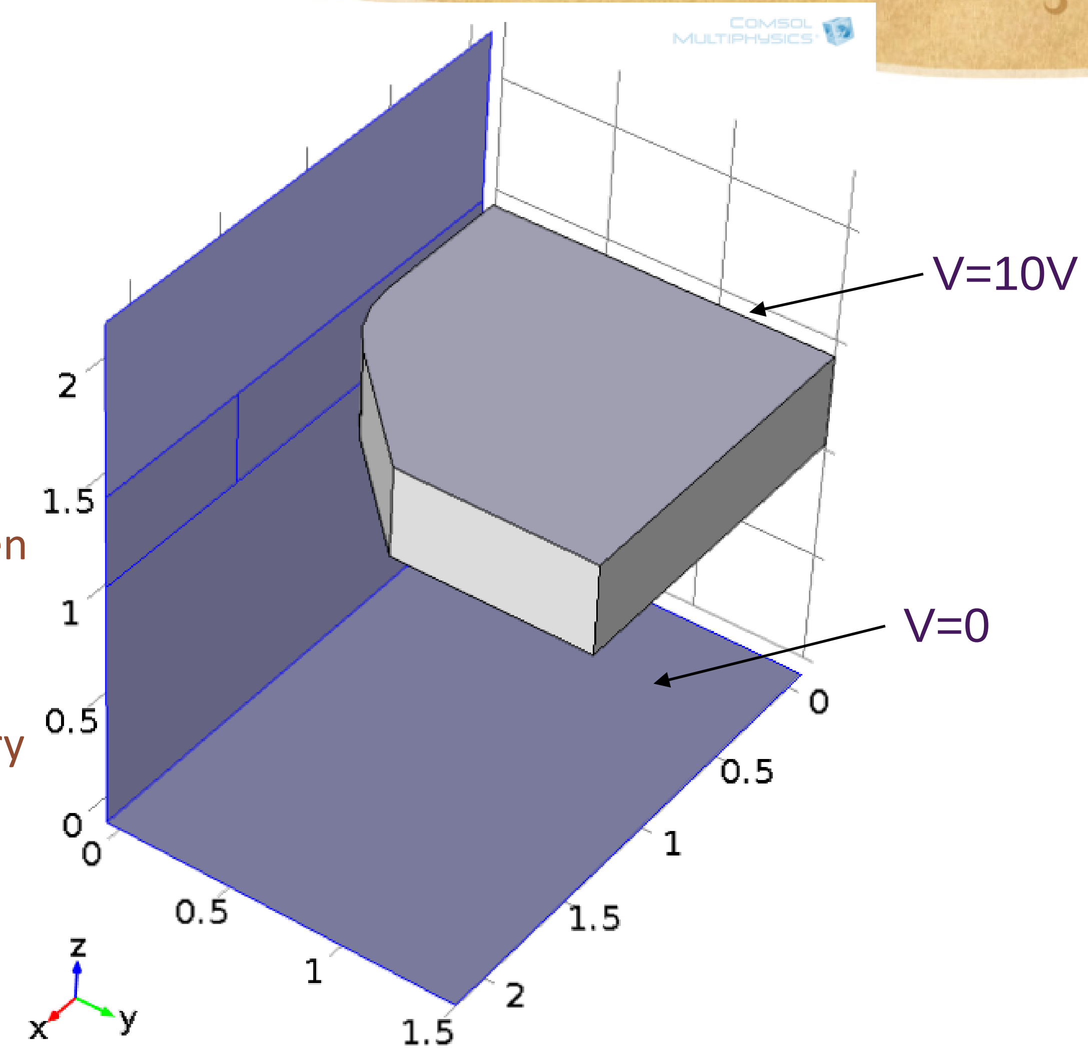
-**Electrostatic regime**

-**Boundary conditions:**

- On the boundary of the electrode: V=10V
- on the Silicon wafer V=0
- on the symmetry plane between the electrodes :

  V=0
- in rest: zero Neumann boundary conditions :

  dV/dn = 0



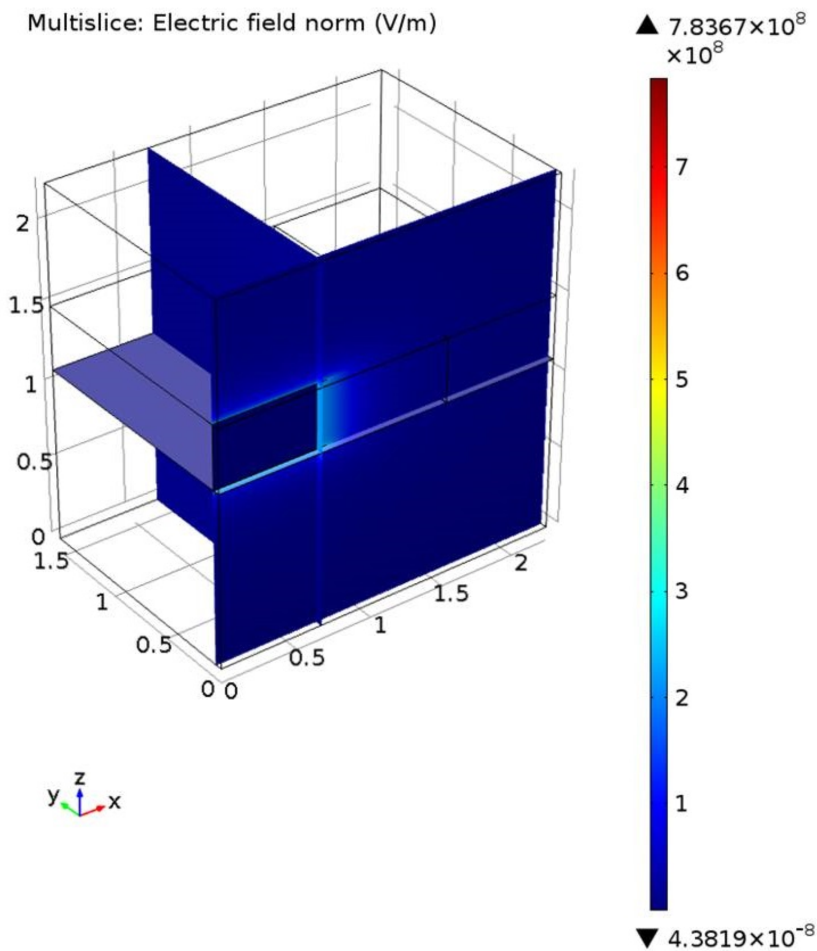
Electric field modeling in the test structure

Transition radius 0

- Degrees of freedom: 26.849.967
- Solving time: 24' 57''
- Used memory: 36.93GB
- E_{max} = 9.3414e8 V/m

Transition radius 10nm

- Degrees of freedom: 23.055.956
- Solving time: 20' 58''
- Used memory: 32.62GB
- E_{max} = 5.6553e8 V/m



A correct estimation of the tunneling current considering the electrostatic edge effect

- **Emax= 214 MV/m (2D top view)**
- **Emax= 1.034 MV/m (2D lateral view)**
- **Emax= 934 MV/m (3D)**

Influence of the sharp edge electrostatic effect on the value of the tunneling current :

E [V/m]	Tr_{WKB}	J [A/m^2]	I [A]
2.149e08	5.34e-80	1.6e-68	5.17e-81
1.034e09	2.8e-17	2e-4	6.4e-17
1.5e09	4.3e-12	64.7	2.07e-11
1.597e09	1.93e-11	319.8	1.023e-10

r_{rac}=1.68e-10m

$$\boxed{I_{measurement} = 2.5 \div 4.4 \cdot 10^{-11}\ A}$$

Conclusions

- Within the nanometric range, the sharp edge electrostatic effect becomes predominant.
- The electric field can not be determined exactly by applying the classic formula E = U/d, thus considering the uniformity of the electric field.
- For $E = 2.149 \cdot 10^8 \mathrm{V/m}$, which represents the value of the electric field intensity obtained according to the classic plane capacitor formula, the WKB approximation gives very small values for the transmission coefficient, current density and tunneling current

Conclusions

- In order to obtain a tunneling current comparable to the measured one, the intensity of the electric field should have a value $\mathrm{E} \approx 1.5 \cdot 10^{9} \mathrm{V/m}$ which is obtained considering a bending radius $r_{rac} = 1.68 \cdot 10^{-10}\, m$.
- A correct estimation of the electrostatic edge effect is obtained only with analytic methods (conformal mapping). These are combined with numeric methods.
- This problem could be solved only by using a multiscale approach.

Thank you!