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```
#%%capture
!pip freeze > requirements.txt
!pip freeze | grep -v -f requirements.txt - | grep -v '^#' | grep -v '^-e ' | xargs pip uninstall -y
```

Abstract

This IV simulation work pertains to performing a Finite Volume Method (FVM, with constant shape function) implementation and a Finite Element Method (FEM, quasi Fermi level with quadratic shape function) implementation of the poisson equation on a 1D (Part I - Part III) / 2D (Part IV) Si pn-diode junction at 293.15K, using COMSOL's 'Multiphysics®' tool.

Rationale for the choice of the two discretization and formulation implementations -

As referred in [1] COMSOL Documentation, FVM discretisation inherently conserves current. Hence FVM provides more accurate charge current results than any other method. However, FEM with quadratic shape function can generate results comparable to FVM, all the while being more computationally efficient with lower degrees of freedom (DOF) in FEM basis formulation. FEM with quasi-Fermi level as the dependent variable (instead of carrier concentration in the FVM case) is advantageous for - systems with wide-bandgaps, systems at very low temperatures, or to include quantum confinement effects.

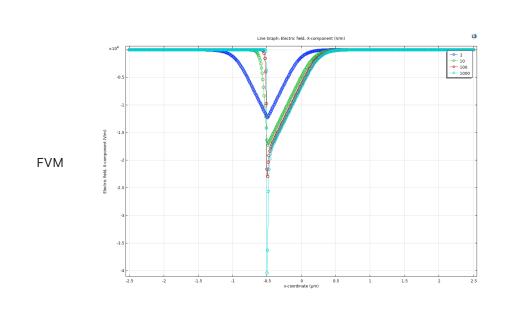
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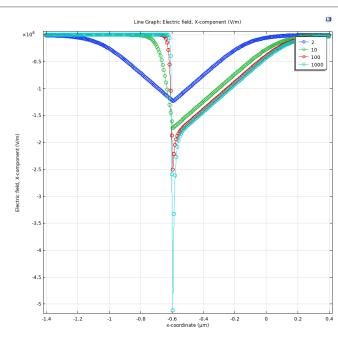
- Part I: Full Depletion vs Depletion approximation
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- Part IV: 2D pn-diode IV sweeps in reverse blocking direction
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Part I: Full Depletion vs Depletion approximation

x = [-2.5:2.5]um, Discretisation points: 500 (Full depletion)

x = [-1.4:0.4]um, R_s = -2.6um, Discretisation points: 250 (Depletion approximation)





Elapsed time (s)

7

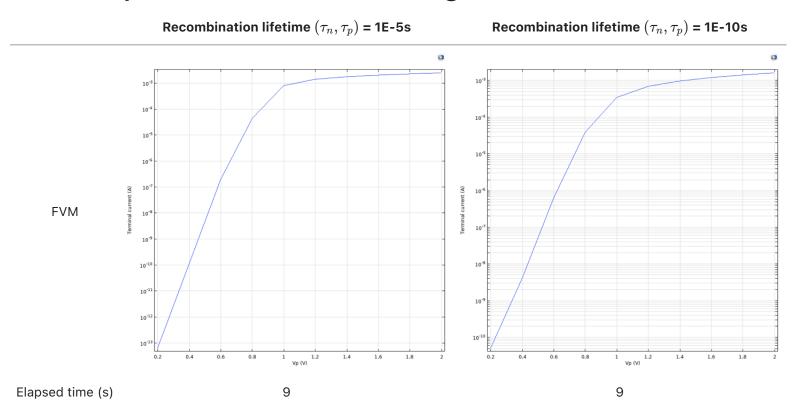
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Summary

1. As can observed in the FVM electric field profile simulation of pn-junction depletion approximation, the elapsed time is shorter due to lesser discretisation points and shorter simulation domain than that of pn-junction full depletion, all the while solving similar electric field profile in the juction region.

2. Henceforth, pn-junction depletion approximation is used for further analysis with a fixed doping ratio (NA/ND) of 1000.

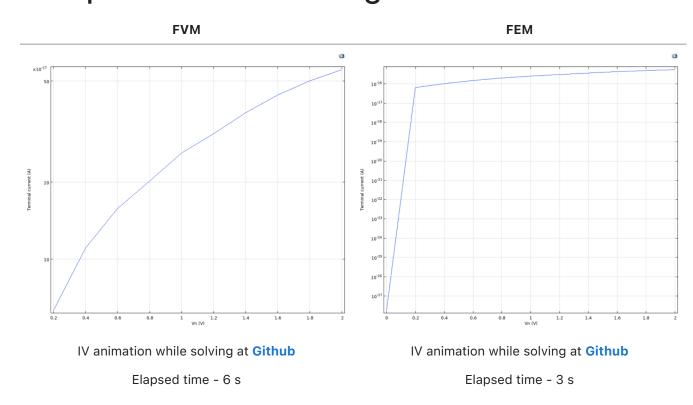
Part II: IV sweeps in forward conducting direction



Summary

- 1. The FVM forward IV sweeps were simulated by accessing current on the p-side terminal (1) while performing an auxiliary sweep of bias on the p-side terminal (1), through a Global Evaluation.
- 2. A Trap-Assisted Recombination node was added to the semiconductor module in the model builder (as referred in [2] COMSOL Documentation), to simulate the effect of a very short carrier recombination lifetime. In the case of τ_n , $\tau_p = 10^{-10} s$, the linear logI-V curve at $V_p = 0.4V$ has a slope change as opposed to a constant slope in the case of normal carrier recombination lifetime $(\tau_n, \tau_p = 10^{-5} s)$. This linear slope change effect is also observed in power MOSFET logI-Vs where carrier recombination lifetime is likewise short.

Part III: IV sweeps in reverse blocking direction

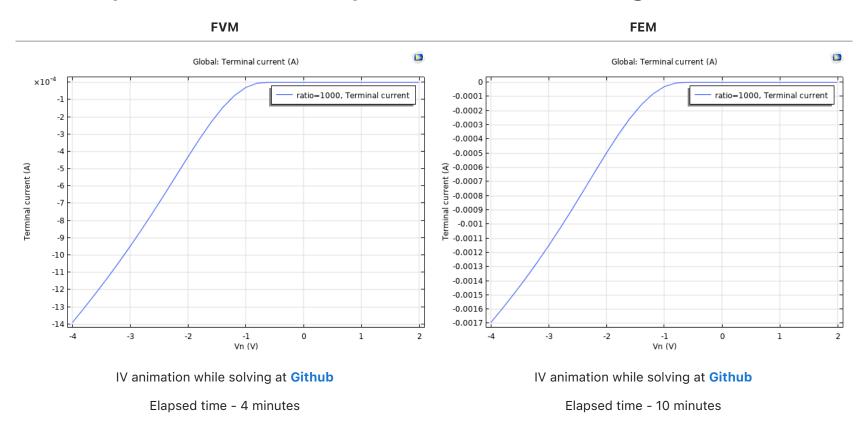


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Summary

- 1. The FVM/FEM reverse IV sweeps were simulated by accessing current on the n-side terminal (2) while performing an auxiliary sweep of bias on the n-side terminal (2), through a Global Evaluation.
- 2. The FVM reverse logI-V curve is smoother (hence more physically reasonable) than the abruptly discrete FEM reverse logI-V curve.
- 3. The 1D FEM reverse IV sweep simulation is faster than the FVM case, which is in-line with the FEM's computational efficiency described in [1] COMSOL Documentation.

Part IV: 2D pn-diode IV sweeps in reverse blocking direction



Summary

- 1. The 2D pn-diode geometry is set up with full junction depletion.
- 2. Just like in Part III, the FVM/FEM reverse IV sweeps were simulated by accessing current on the n-side terminal (2) while performing an auxiliary sweep of bias on the n-side terminal (2), through a Global Evaluation.
- 3. Unlike in the 1D case, the 2D FVM and FEM reverse IV sweeps are nearly identical, which is due to the finer mesh selection (greater discretisation of 2D geometry) used in both FVM and FEM simulations.
- 4. Interestingly, the 2D FVM reverse IV sweep simulation is faster than the FEM case, which is due to higher DOF in FEM basis formulation for the 2D finer mesh (246123 in FEM vs 60000 in FVM).

References

- [1] COMSOL Documentation Discretization and Formulation Options
- [2] COMSOL Documentation P-N Junction 1D

Additional information

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Data and config file at: Github