Efficient Optical Modeling of Graphene

in FDTD Solutions and MODE Solutions

LUMERICAL SOLUTIONS INC.

Outline

Introduction

- Lumerical's optical simulation products
- Physical properties of graphene

New Graphene Modeling Workflow

- New surface conductivity model
- New surface geometric primitive
- Simple example: transmission through a graphene sheet

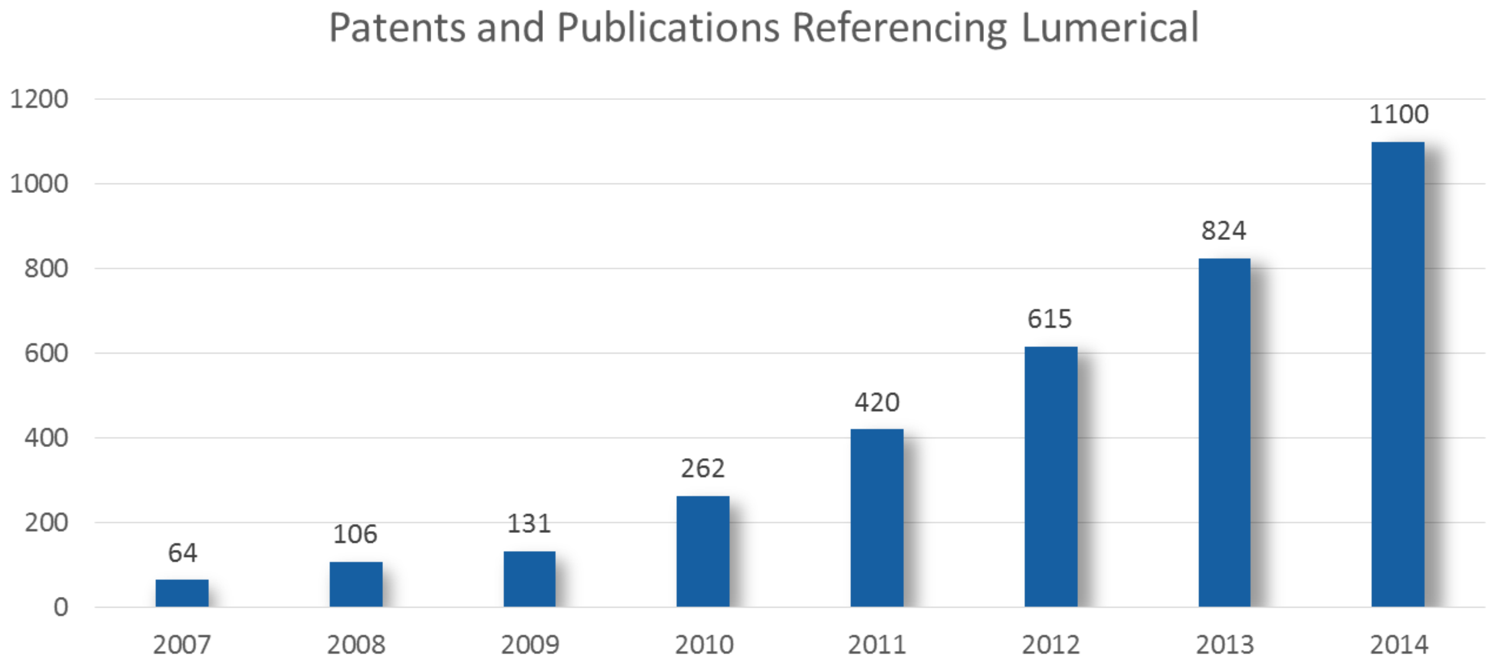
Application Examples

- Tunable THz metamaterial (FDTD)
- Graphene waveguide modulator (FDTD and MODE)
- Exciting a surface plasmon mode (FDTD and MODE)

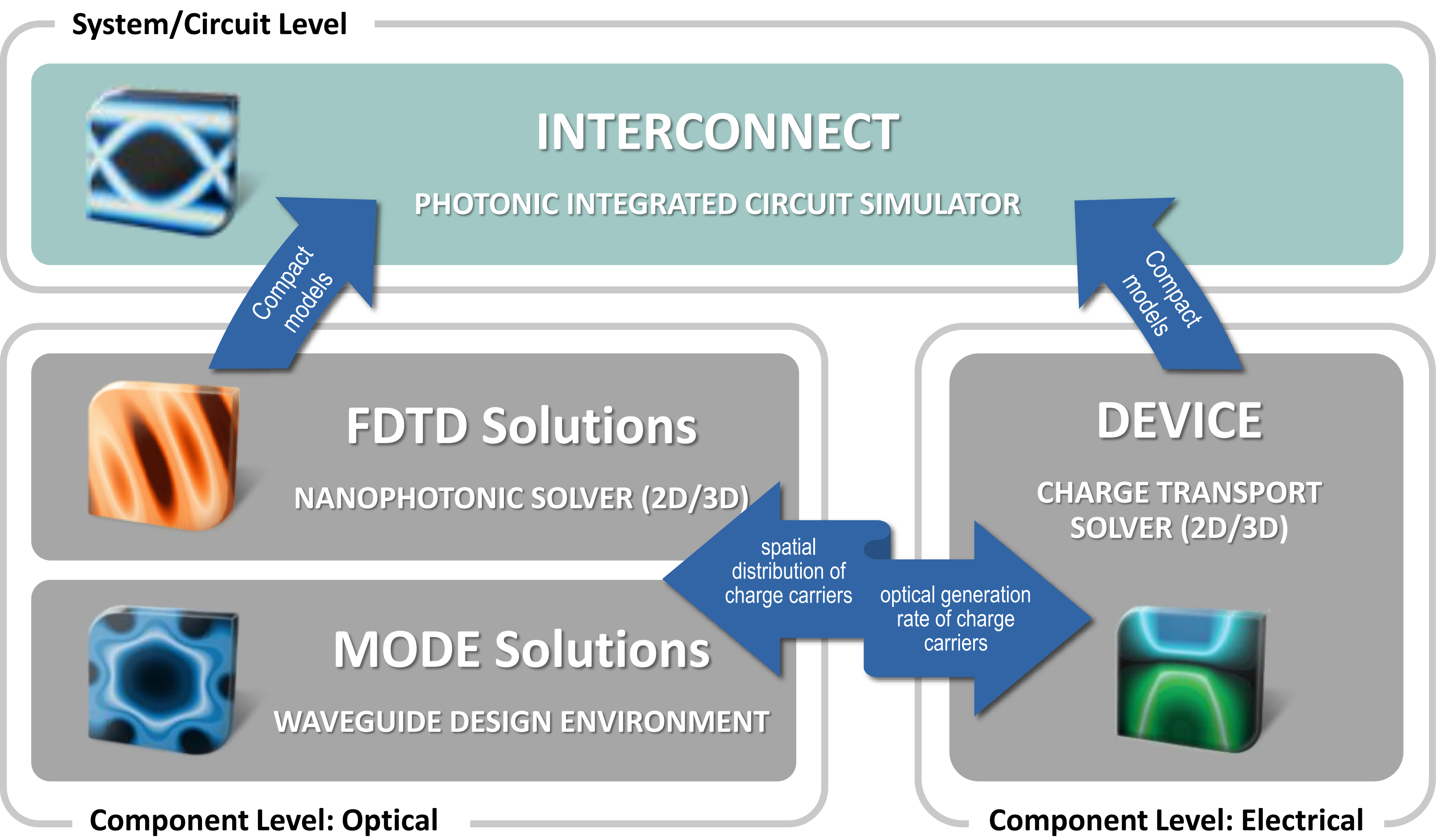
Summary

Lumerical Solutions

Lumerical empowers R&D professionals with best-in-class design tools and services to support the creation of better photonic technologies



Our Products



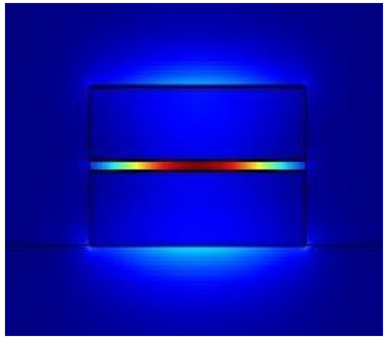
Lumerical's Optical Solvers

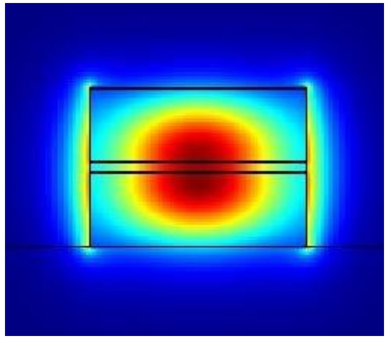
MODE Solutions

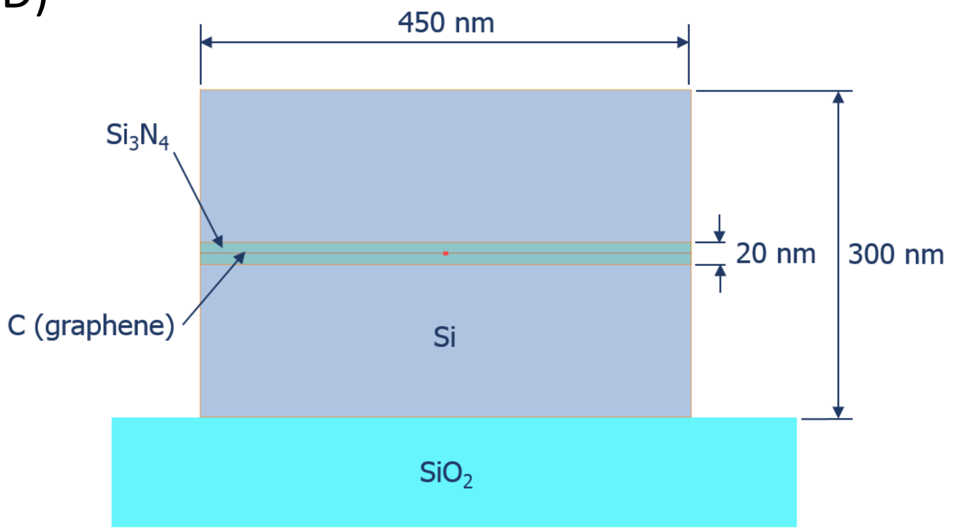
- Finite difference eigenmode solver (FDE)
- Bidirectional eigenmode expansion solver (EME)
- 2.5-D variational finite difference time domain solver (varFDTD)

FDTD Solutions

- 2-D and 3-D finite difference time domain solver (FDTD)



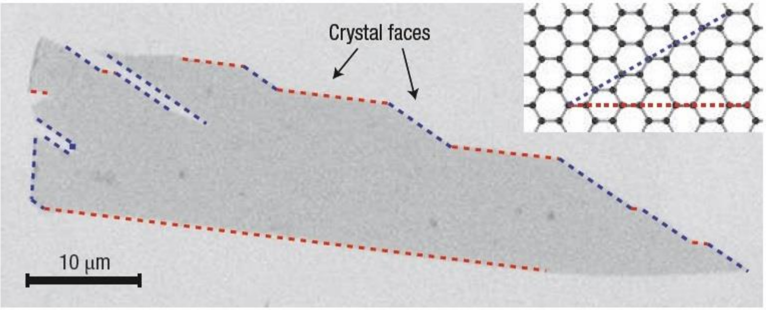




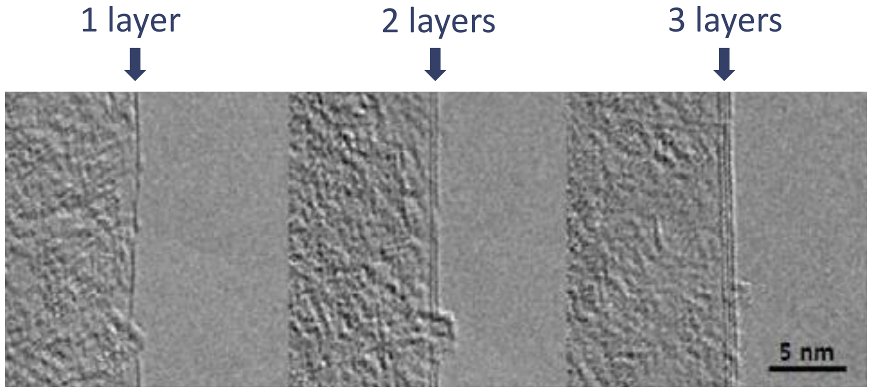
Graphene's Physics

What makes graphene different from other optical materials?

- It is a truly 2-D material:



[1] A.K. Geim and K.S. Novoselov, “The rise of graphene," *Nature Materials*, vol. 6, pp. 183-191, 2007.



[2] S. Bae *et al.*, “Roll-to-roll production of 30-inch graphene films for transparent electrodes," *Nature Nanotechnology*, vol. 5, pp. 574-578, 2010.

Graphene's Physics

Graphene is usually modeled using a surface conductivity:

$$\sigma(\omega,\Gamma,\mu_c,T) = -\frac{ie^2(\omega+i2\Gamma)}{\pi h^2}\left[\frac{1}{(\omega+i2\Gamma)^2}\int_0^\infty \epsilon\left(\frac{\partial f_d(\epsilon)}{\partial\epsilon} - \frac{\partial f_d(-\epsilon)}{\partial\epsilon}\right)d\epsilon - \int_0^\infty \frac{f_d(-\epsilon)-f_d(\epsilon)}{(\omega+i2\Gamma)^2-4(\epsilon/\hbar)^2}d\epsilon\right]$$

$$f_d(\epsilon) = \left(e^{(\epsilon-\mu_c)/(k_BT)}+1\right)^{-1}$$

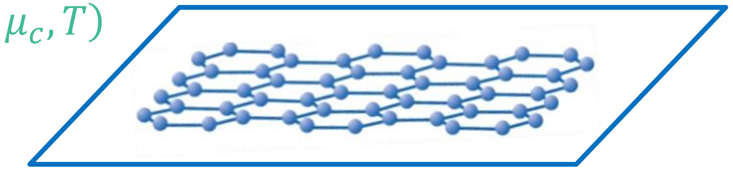
intraband **interband**

[3] G. Hanson, "Dyadic Green's functions and guided surface waves for a surface conductivity model of graphene", *Journal of Applied Physics*, vol. 103 (64302), 2008.

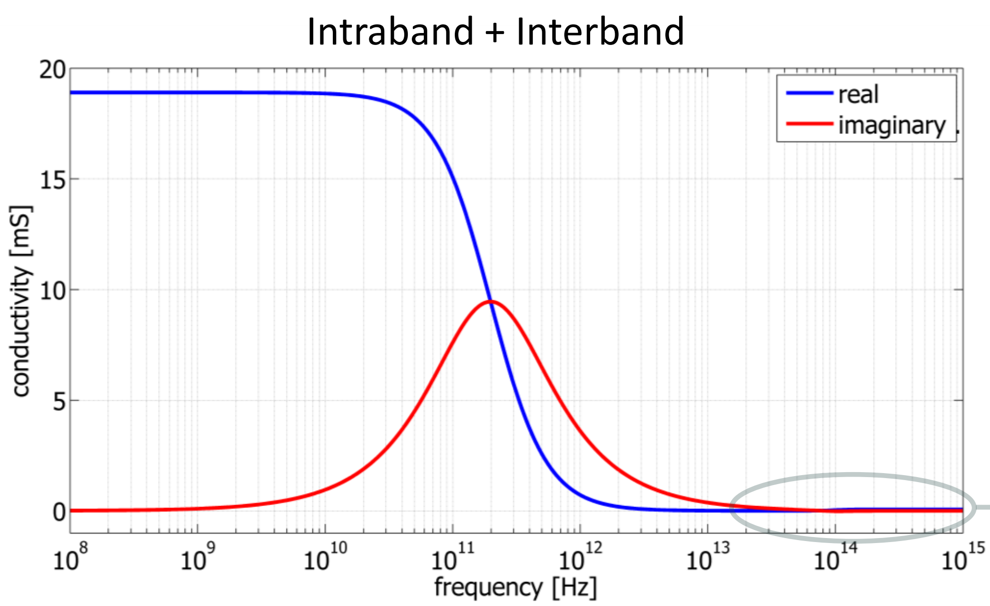
The new workflow is based on a surface conductivity model

- Two new components have been added to the UI in FDTD and MODE:
  - a new surface conductivity model,
  - and a new surface primitive.

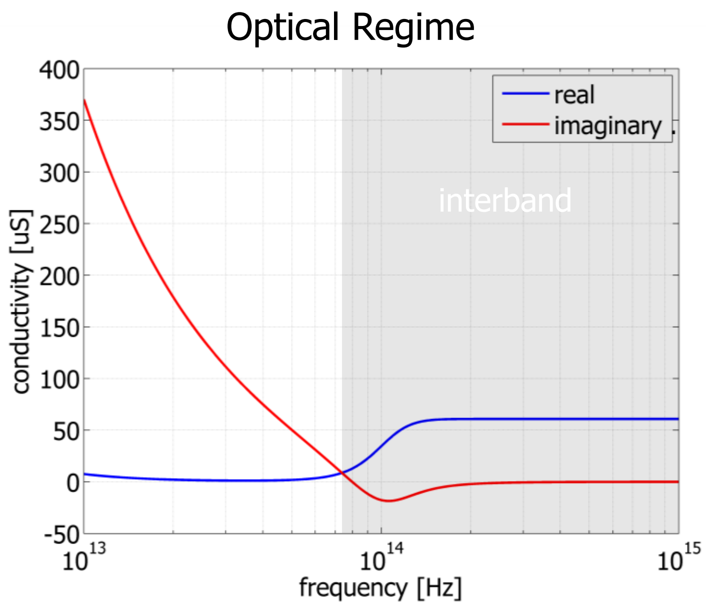
$\sigma(\omega,\Gamma,\mu_c,T)$



Surface Conductivity of Graphene



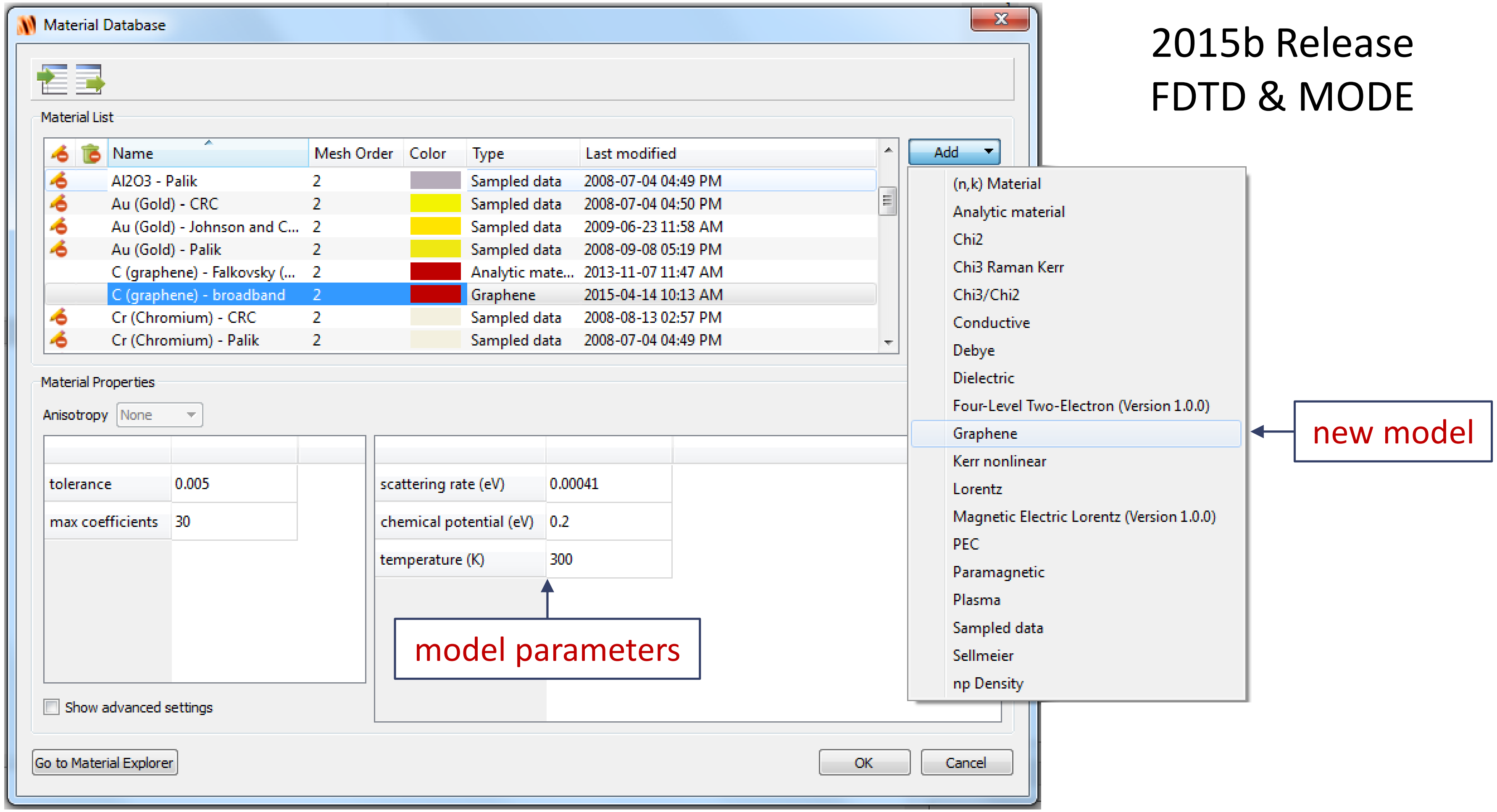
$\Gamma = 0.41\mathrm{meV}$
$\mu_c = 0.2\mathrm{eV}$
$T = 300\mathrm{K}$



Notes

- Intraband term dominates at low frequencies.
- Interband term dominates at optical frequencies.
- Interband term must be obtained numerically.

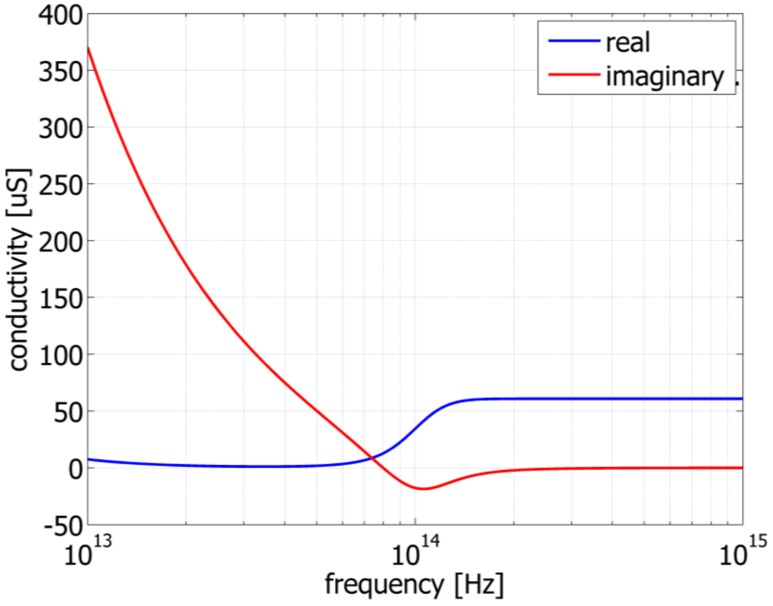
New Surface Conductivity Model

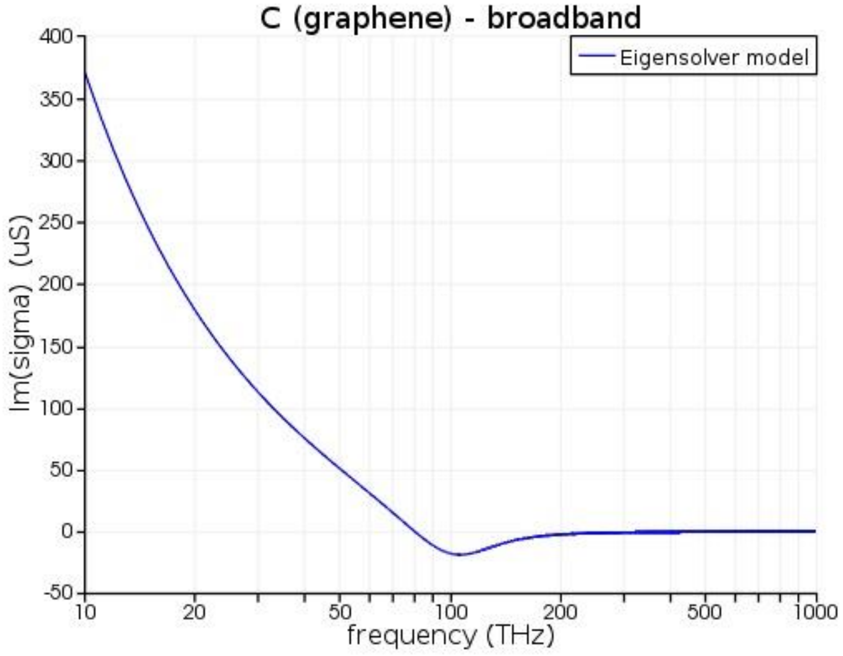


2015b Release

FDTD & MODE

Generating Conductivity Plots





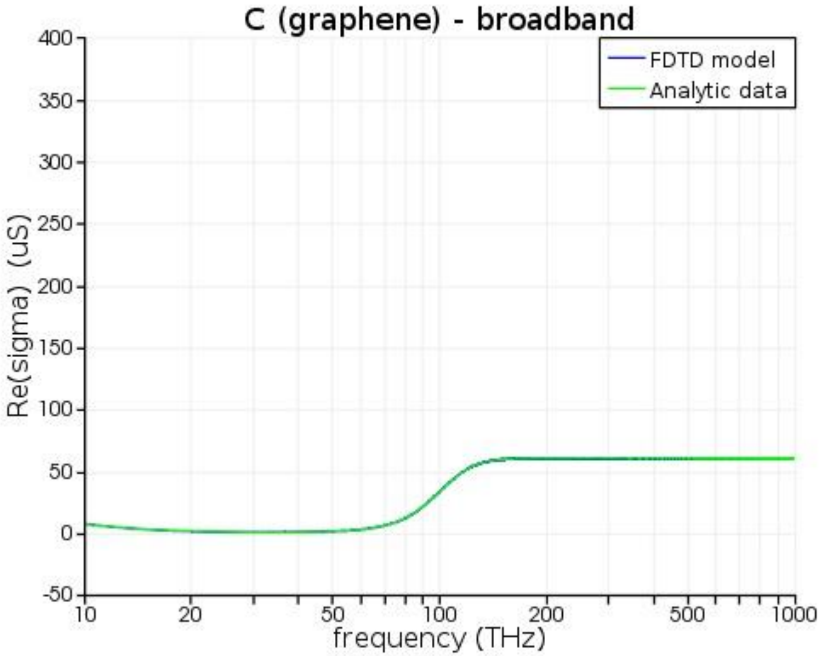
Notes

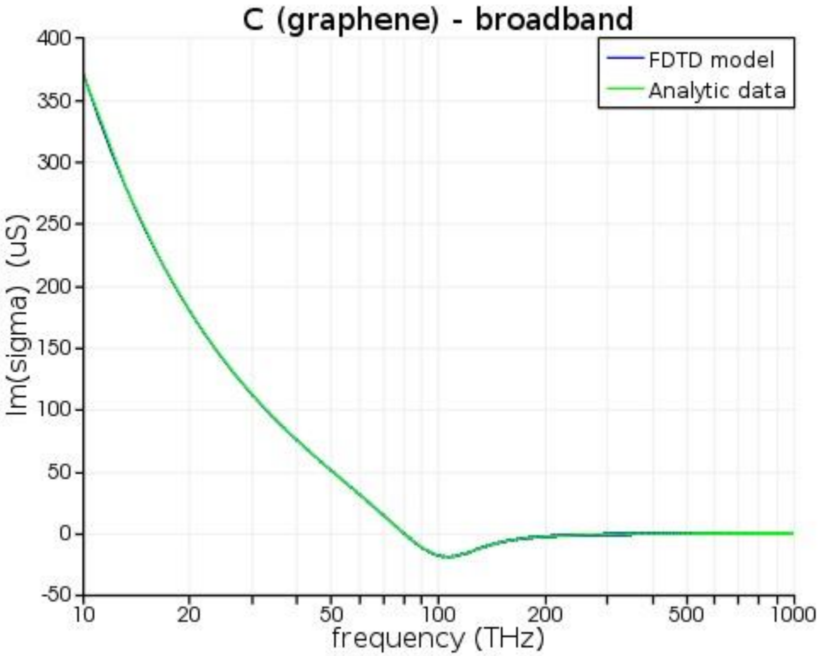
- Brief demonstration: how to generate surface conductivity plots.
- Interband integral is computed numerically.

New Surface Conductivity Model in FDTD

FDTD Solutions needs a multi-coefficient material (MCM) model

- FDTD Solutions creates a multi-coefficient model of the surface conductivity.
- This model can be compared with the surface conductivity data.





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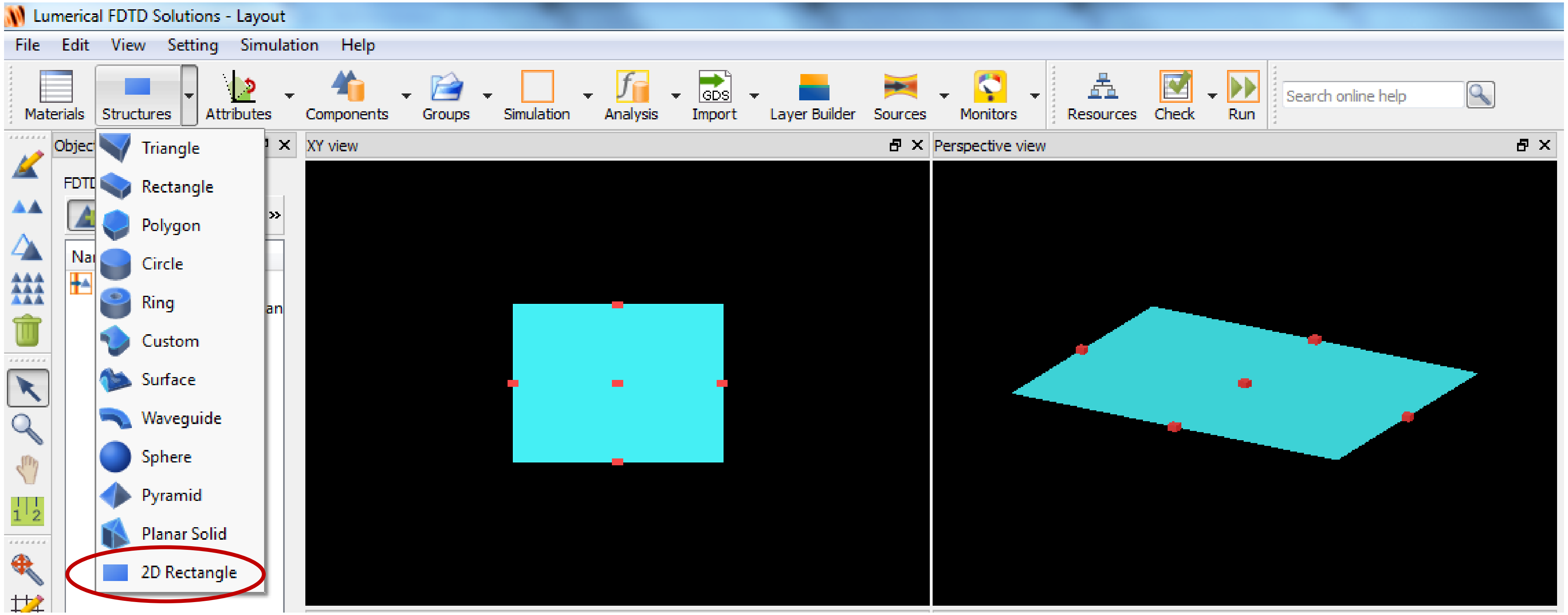
New Surface Primitive

FDTD 2015B Release

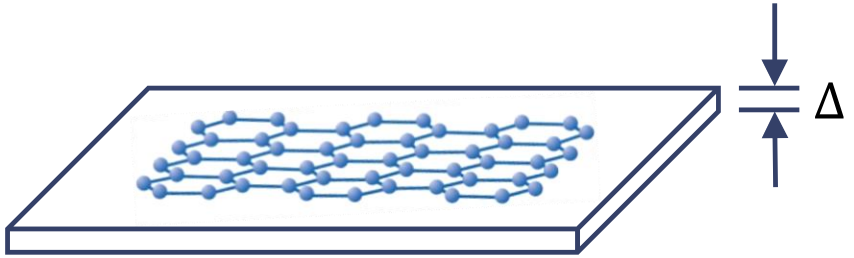


- The new 2D rectangle was specifically created for modeling graphene.
- The surface normal vector must be parallel to one of the three coordinate axes.

New Graphene Modeling Workflow

A surface conductivity can be turned into a volumetric permittivity:

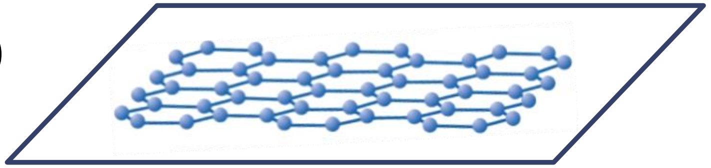
$$\varepsilon(\omega) = \varepsilon_0\varepsilon_r + i\,\frac{\sigma(\omega)}{\omega\Delta}$$



- A volumetric permittivity model is currently employed in FDTD and MODE.

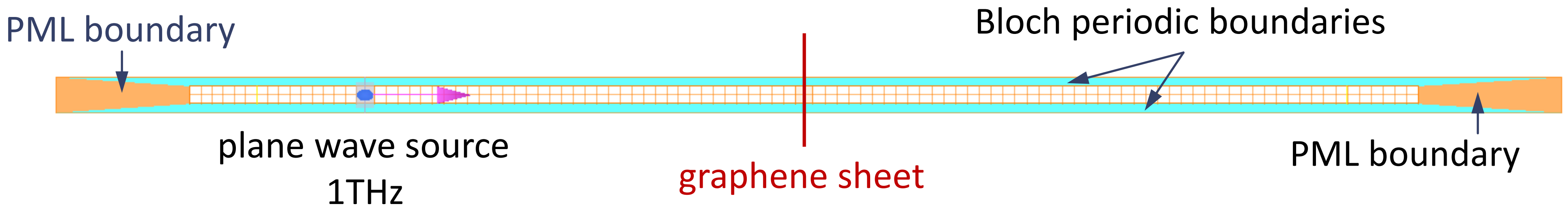
The new workflow is based on a surface conductivity model:

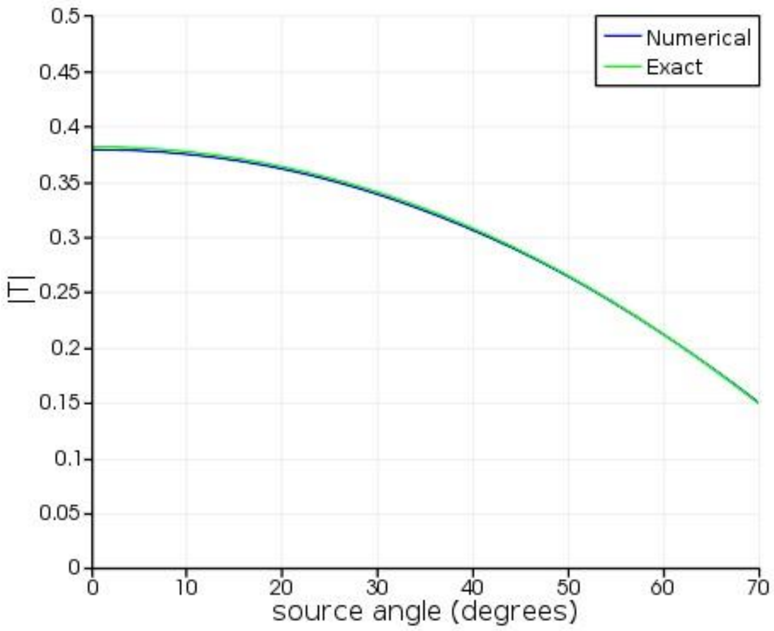
$\sigma(\omega)$

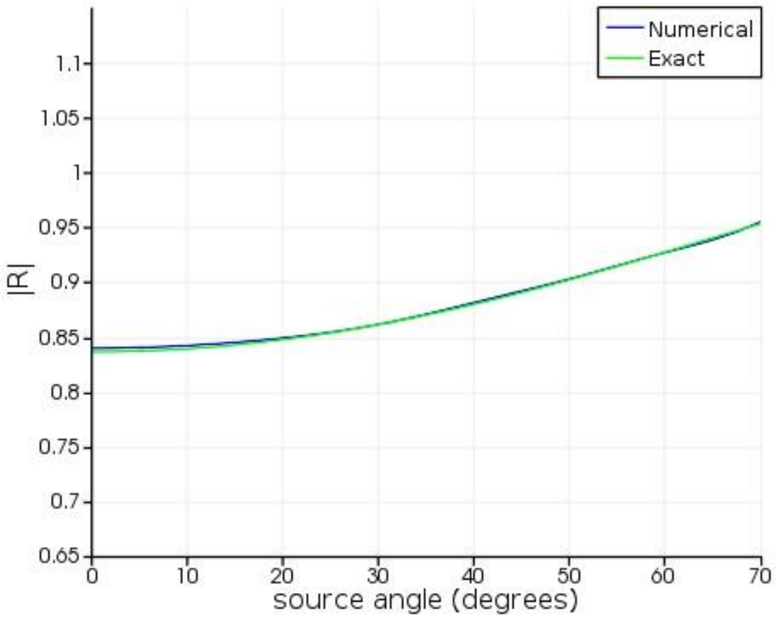


- New UI components: a surface conductivity model, and a surface primitive.

Plane Wave Transmission / Reflection

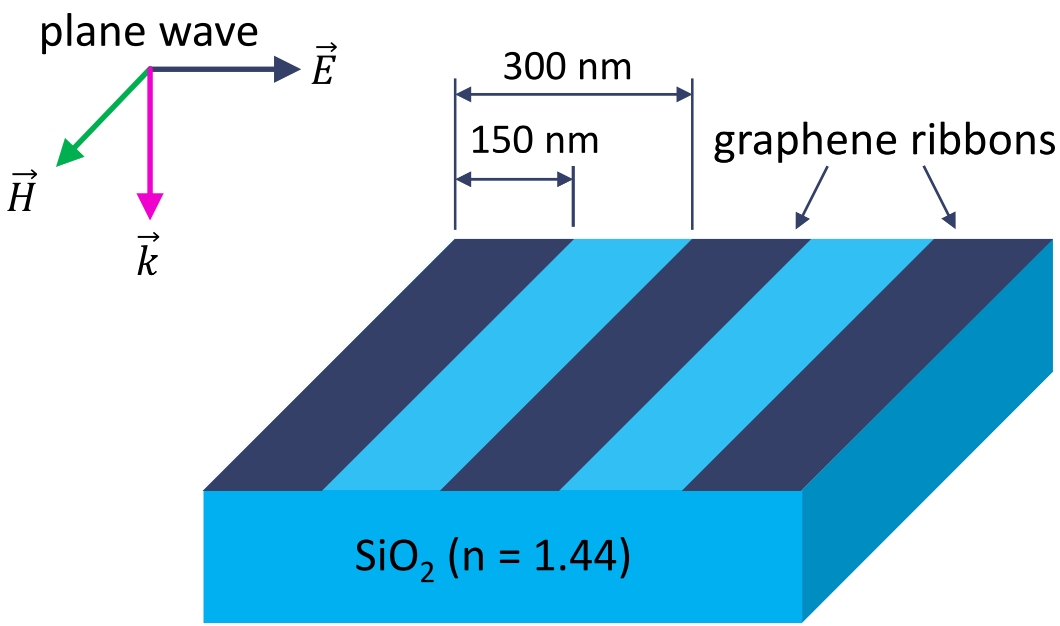






Tunable THz Metamaterial

Graphene ribbons deposited on a dielectric substrate:

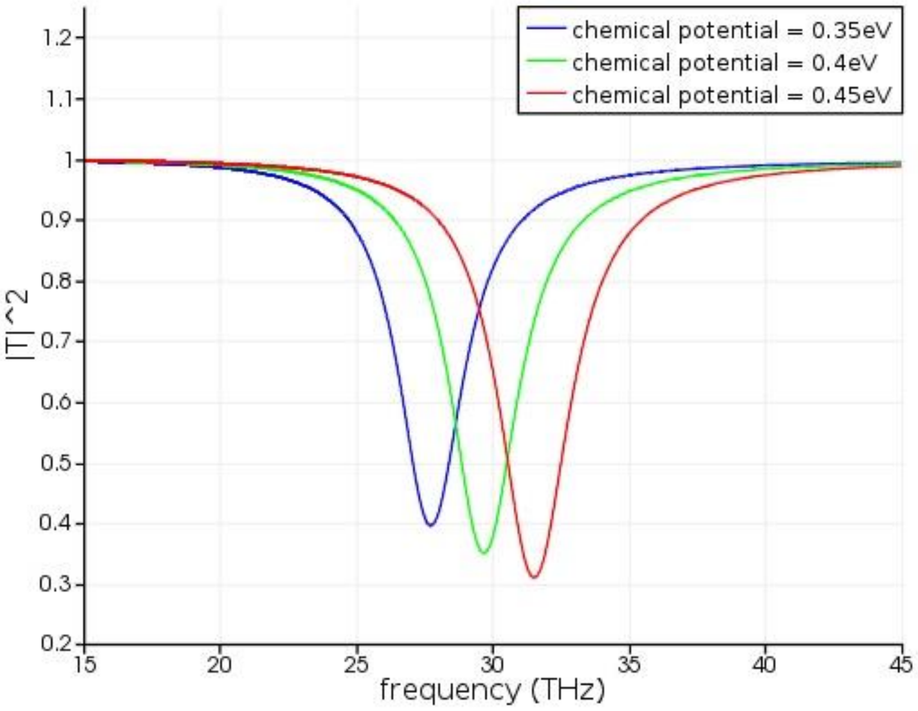


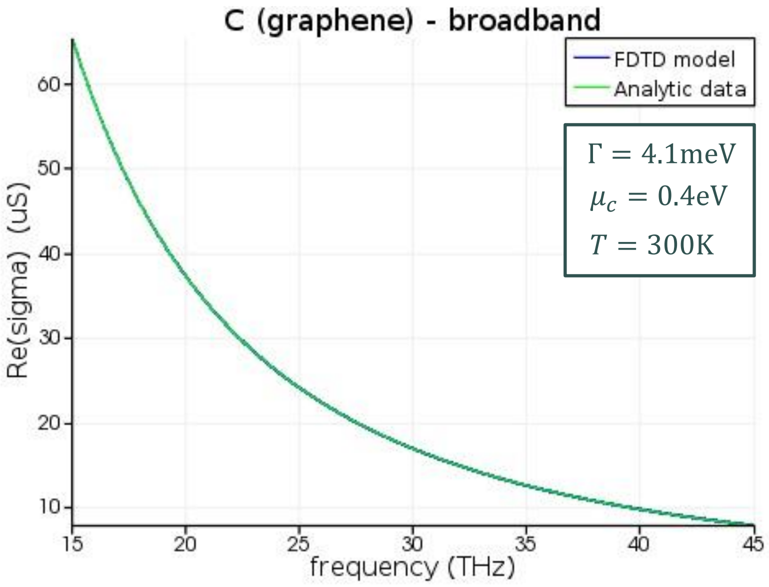
- Chemical potential of the ribbons can be tuned using a voltage source.
- The FDTD solver can produce broadband results thanks to the MCM model.

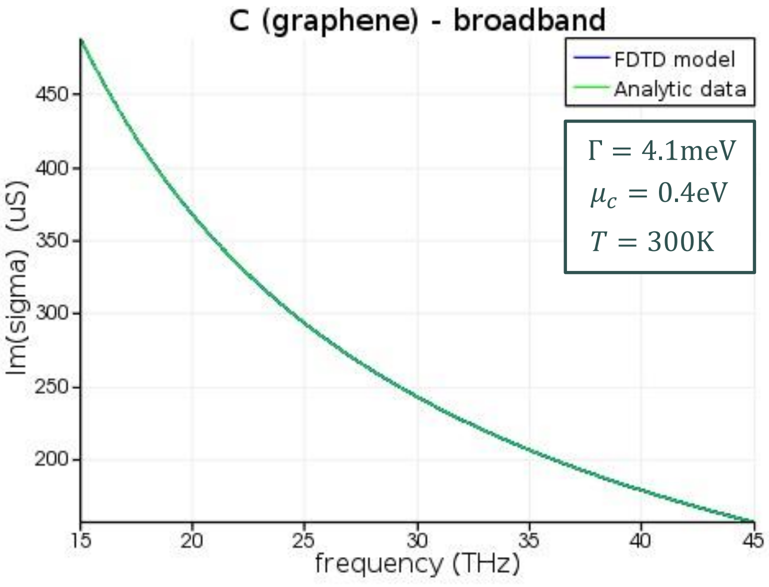
[4] H. Chu and C. Gan, "Active plasmonic switching at mid-infrared wavelengths with graphene ribbon arrays," *Applied Physics Letters*, vol. 102 (231107), 2013.

Tunable THz Metamaterial

Transmitted Power Without Substrate

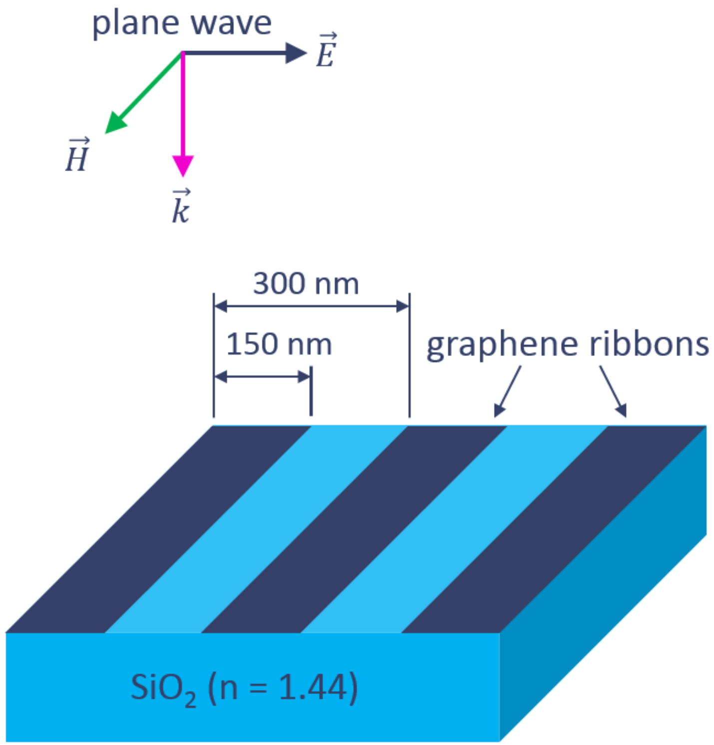




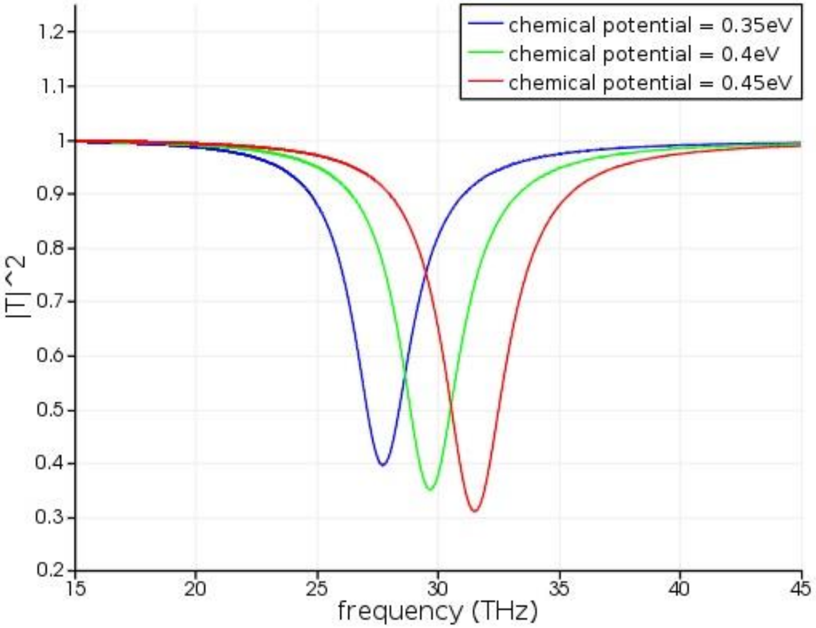


method	min mesh size	time
new	2.5 nm	67s
old	0.1 nm	1h+7min

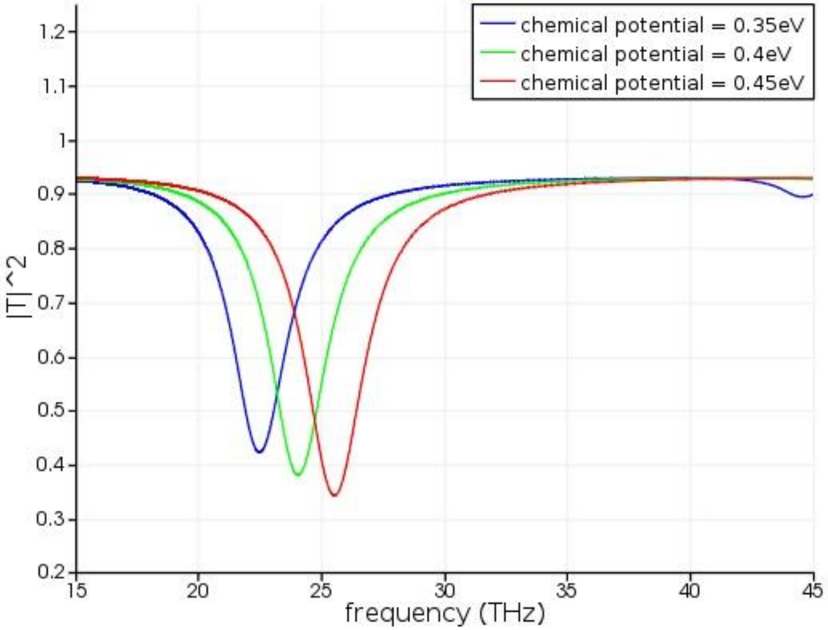
Tunable THz Metamaterial



Transmitted Power Without Substrate

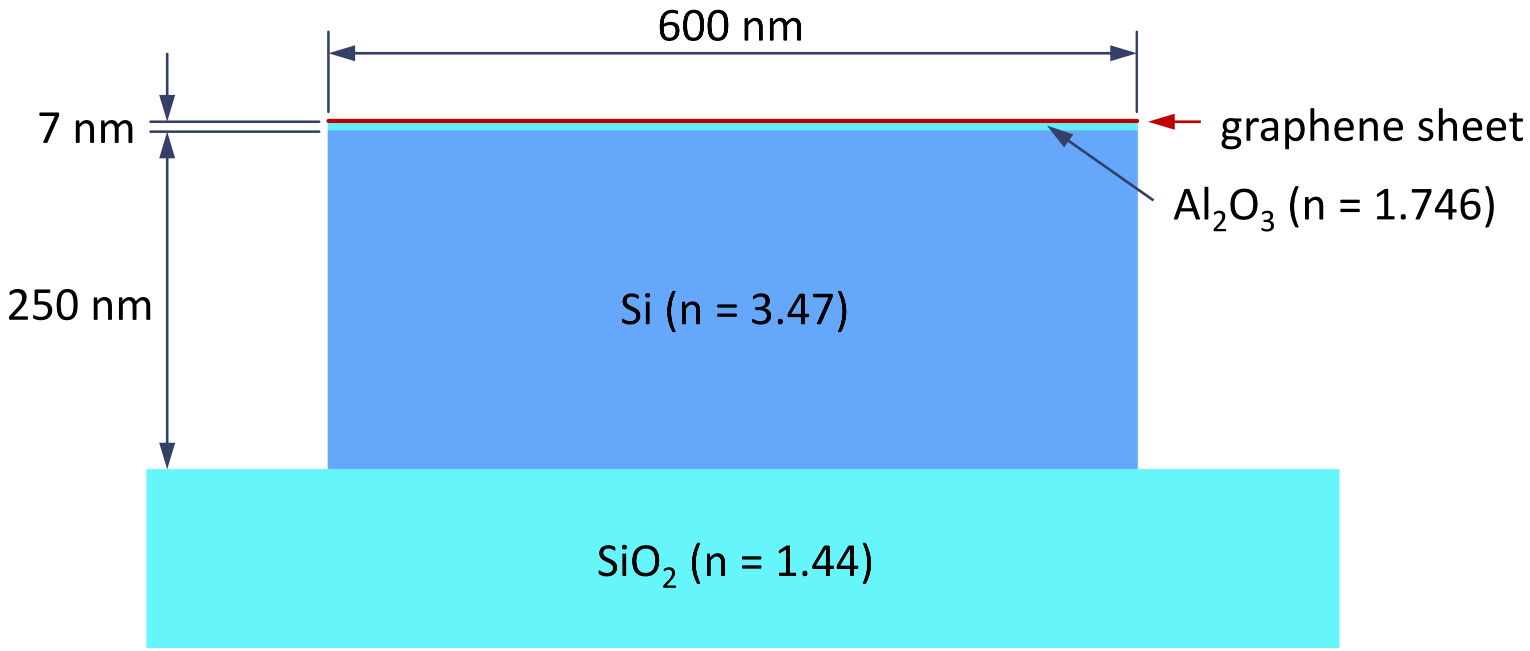


Transmitted Power With Substrate

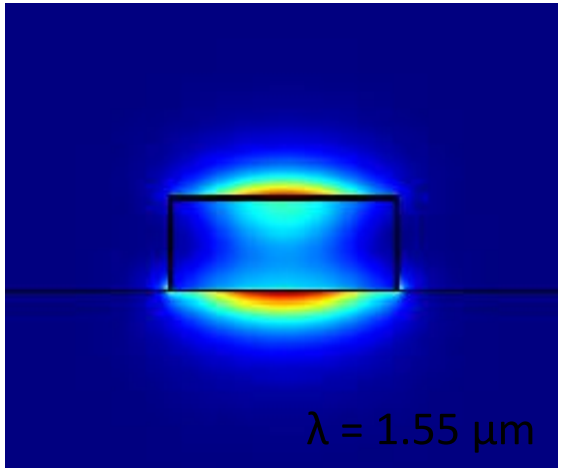


Electro-Optical Modulator

Based on the following waveguide configuration:



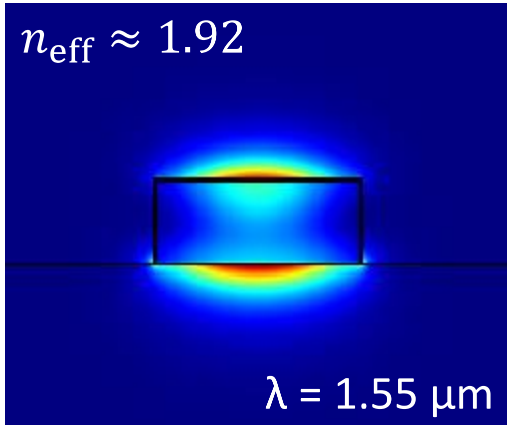
Desired Mode

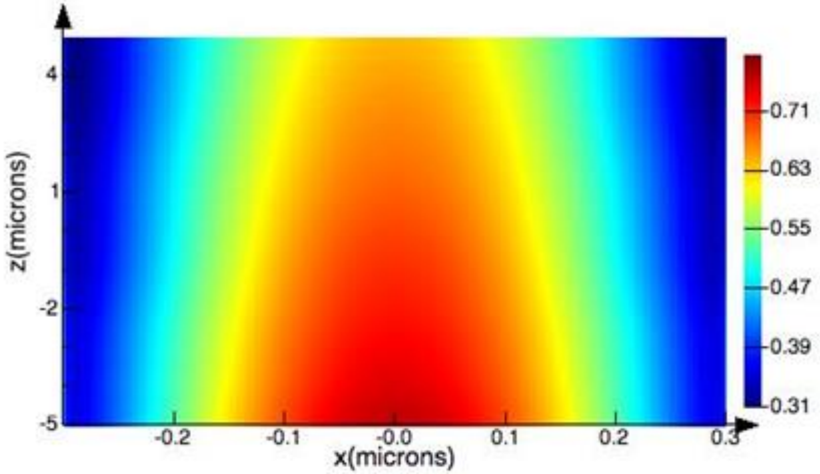


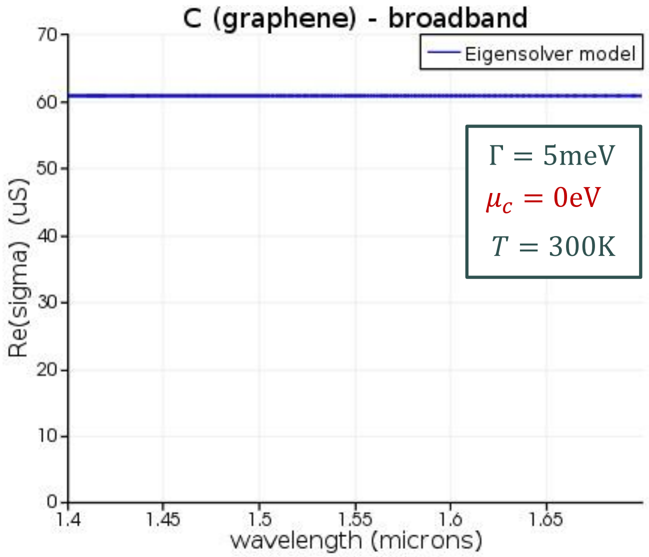
- Chemical potential of the graphene layer can be tuned using a voltage source.
- The shown waveguide mode was obtained using the FDE solver.

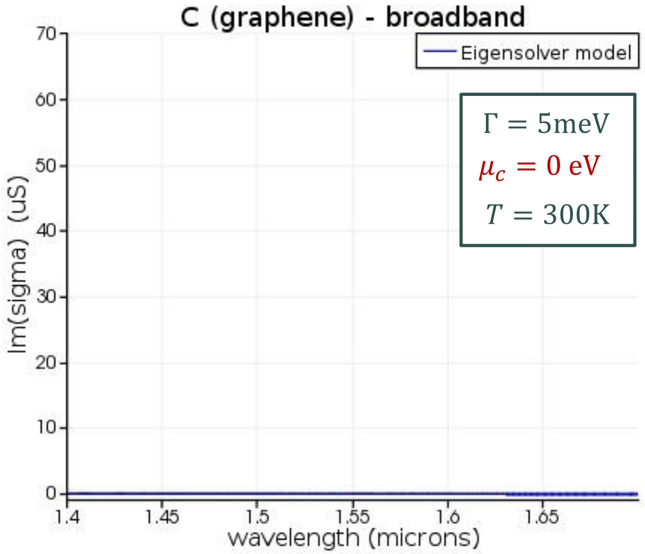
[5] M. Liu, X. Yin, E. Ulin-Avila, B. Geng, T. Zentgraf, L. Ju, F. Wang and X. Zhang , "A graphene-based broadband optical modulator", *Nature Letters*, vol. 474, pp. 64-67, 2011.

Electro-Optical Modulator – Off State





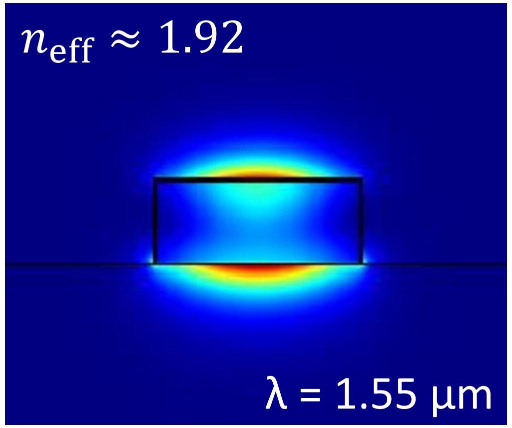


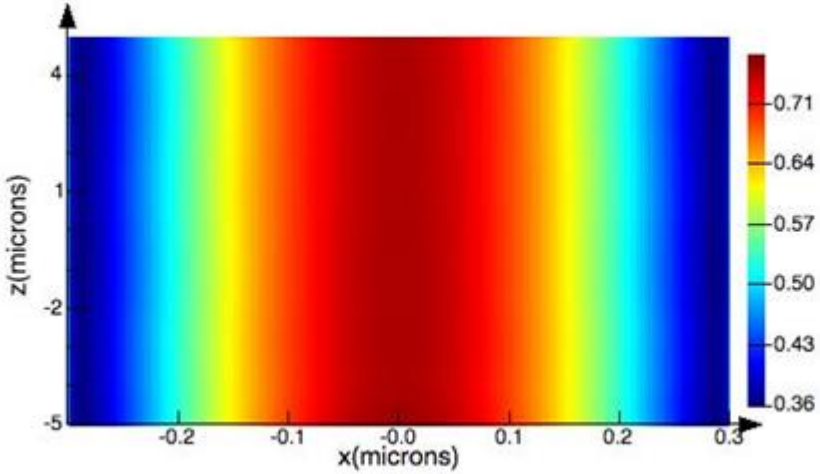


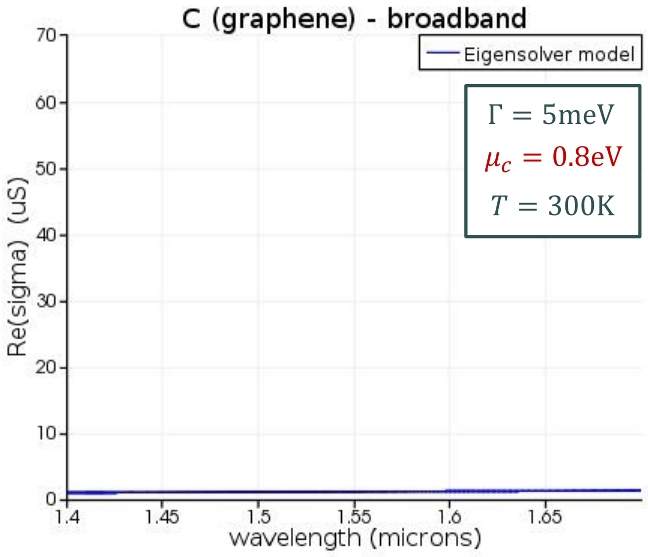
Loss $= 0.148$ dB/µm

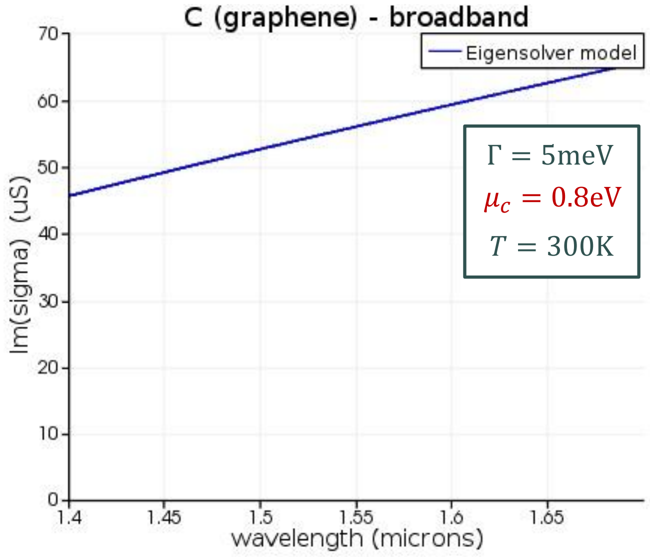
- When the chemical potential is zero, the loss is high enough to attenuate the waveguide mode significantly.

Electro-Optical Modulator – On State









Loss $= 0.0032$ dB/μm

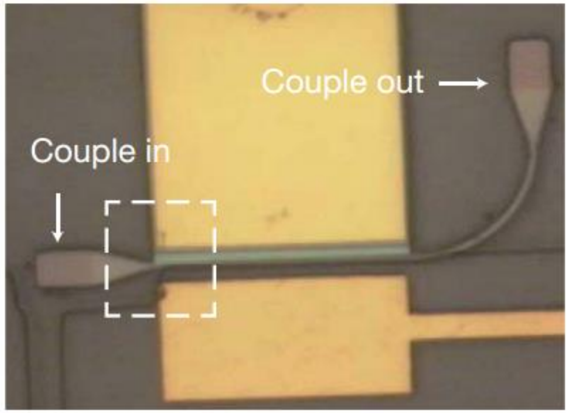
- When the chemical potential is 0.8 eV, the loss is low and there is virtually no attenuation of the waveguide mode.

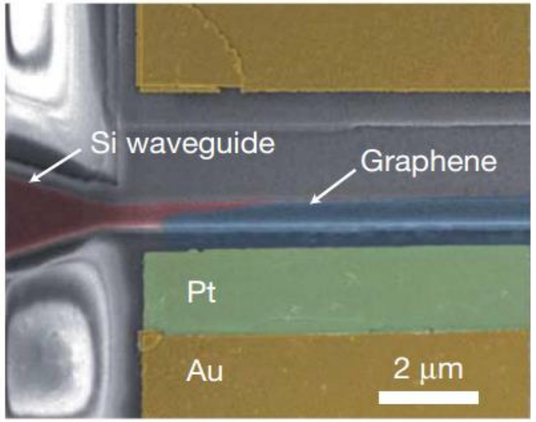
Electro-Optical Modulator

FDTD Speed-up:

method	time
new	39 min
old	2h+15min

Prototype:





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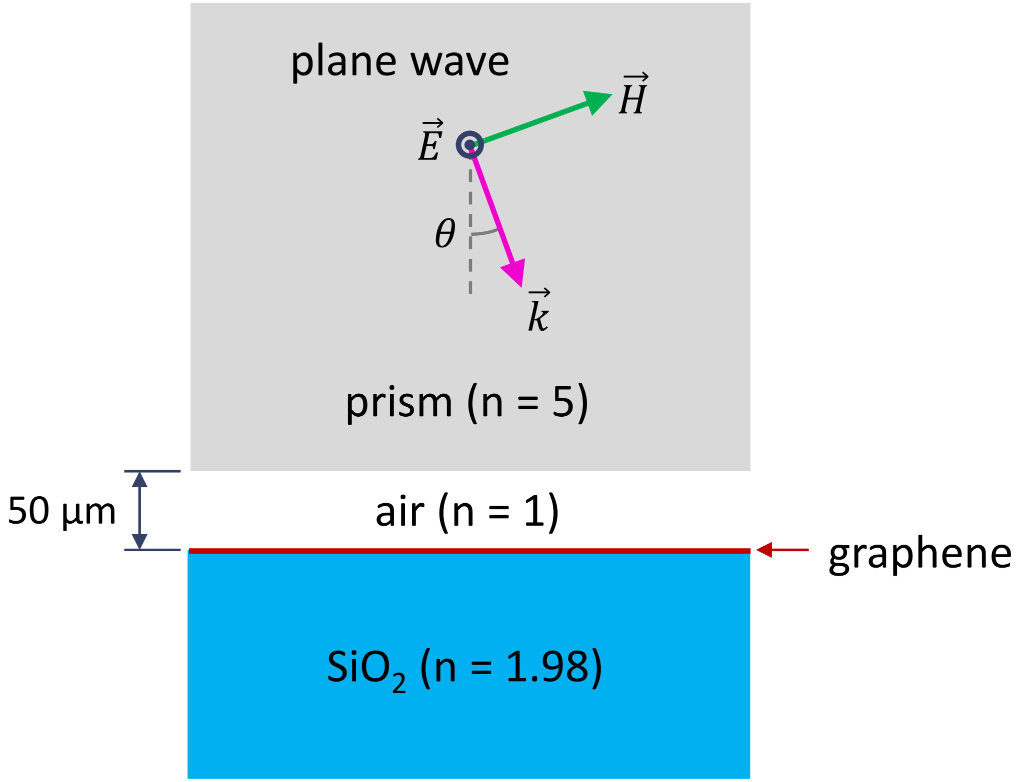
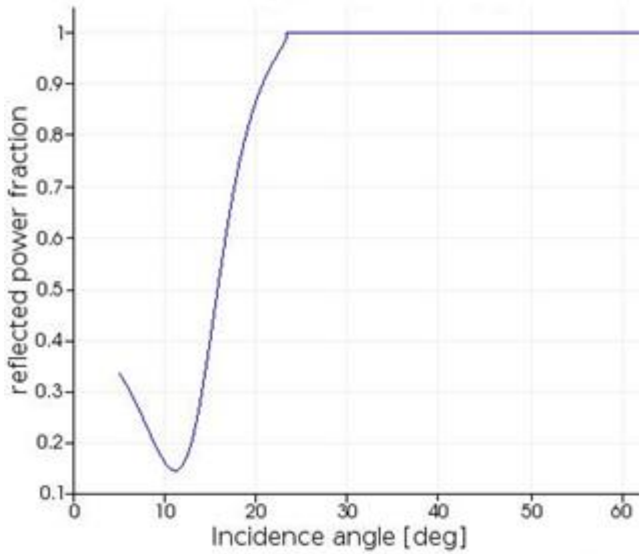
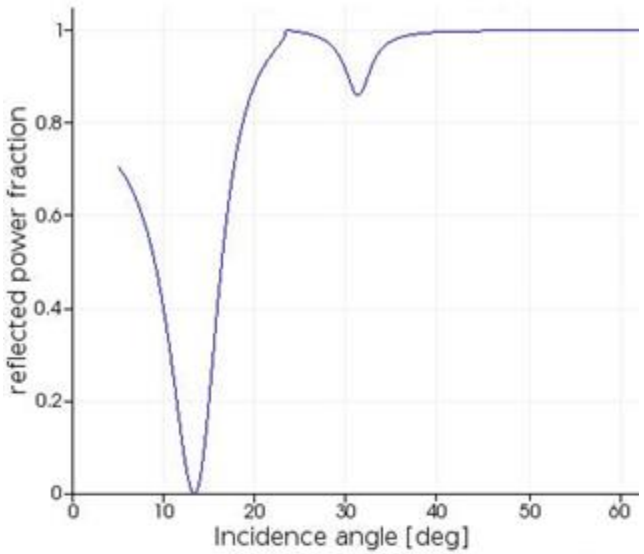
Exciting a Surface Plasmon Mode

Light at 0.5 THz incident from a prism:







- At $\theta \approx 31°$, a surface plasmon (SP) is excited.
- Exact results obtained with the transfer matrix method.

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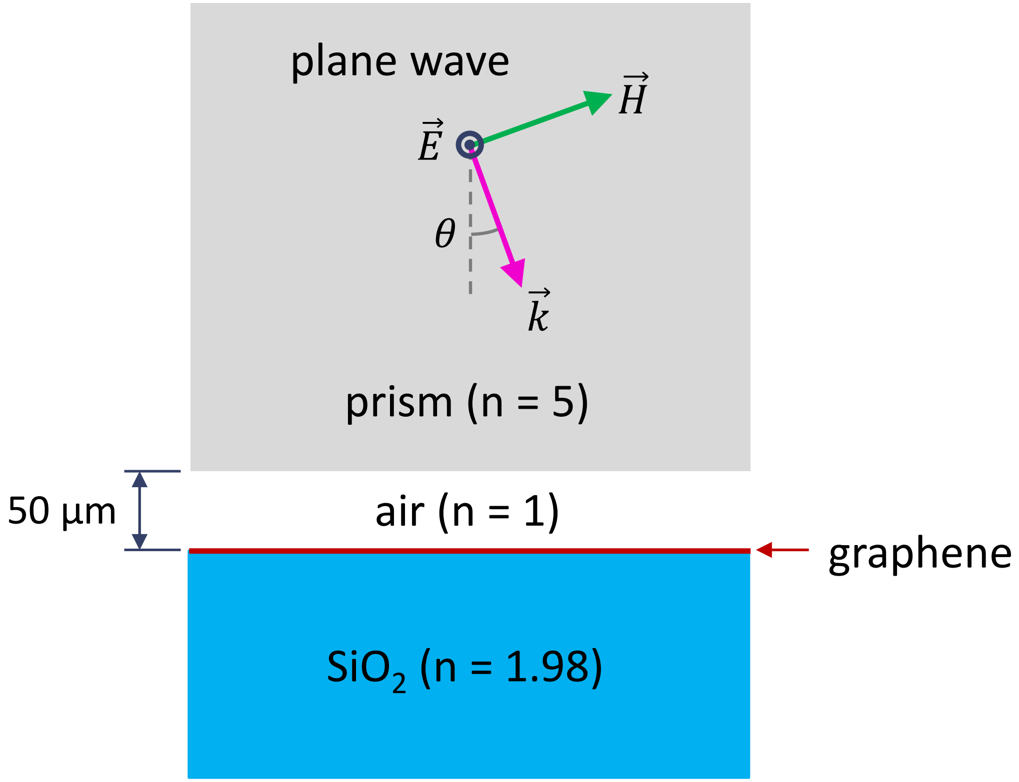
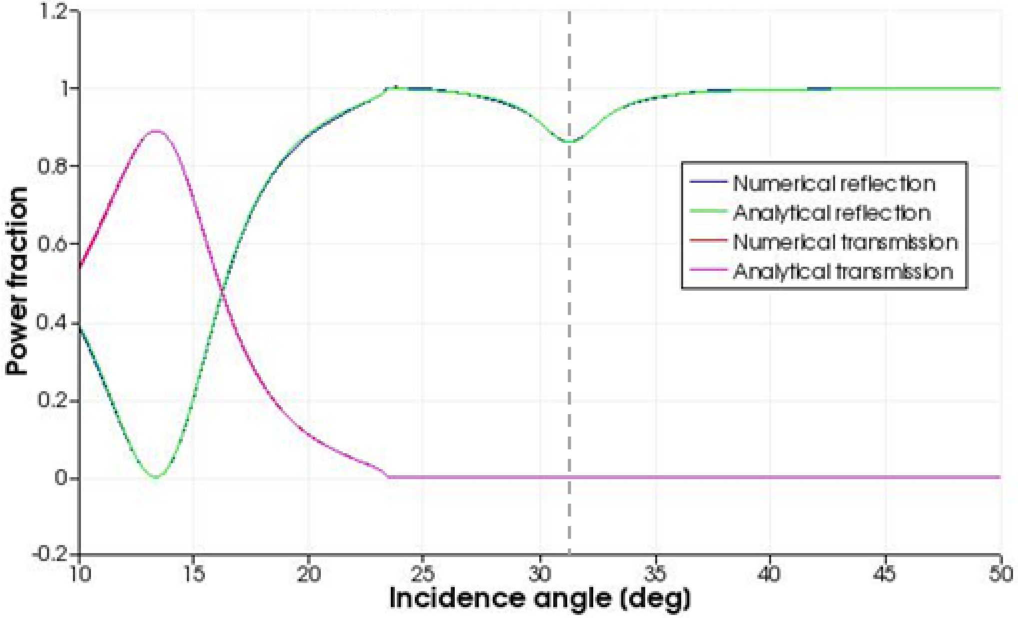
Exciting a Surface Plasmon Mode

Light at 0.5 THz incident from a prism:



Numerical vs. Analytic



- The SP mode can also be modeled using the FDE solver:

$$n_{\text{eff}} = 2.5625 + i0.1202 \qquad \theta = \sin^{-1}(\text{Re}(n_{\text{eff}})/5) \approx 30.8°$$

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Summary

- **Improved graphene workflow available in FDTD and MODE (2015B)**
- **Graphene is now treated as a 2-D material**
  - A new surface conductivity model is being introduced.
  - A new geometric primitive specifically for graphene.
- **Treating graphene as a 2-D material leads to faster simulations**

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