MULTIPHYSICS SIMULATION

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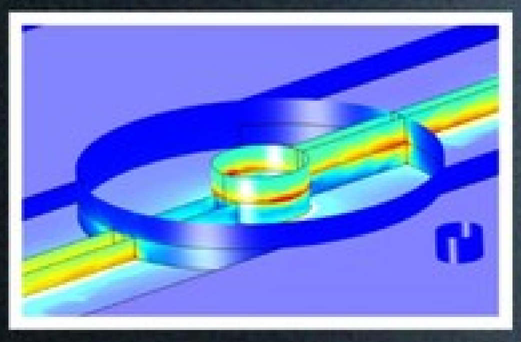


INTEL IMPROVES SIGNAL INTEGRITY AND SPEED
PAGE 18

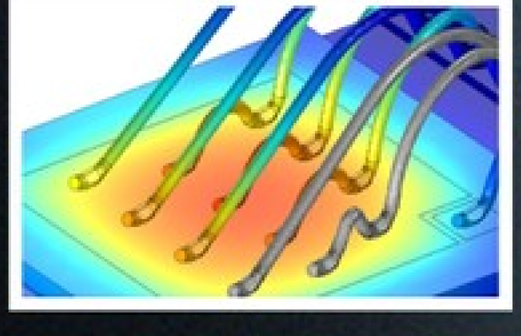


ABB EXTENDS LIFETIME OF POWER TRANSISTORS
PAGE 20

SIMULATION POWERS WIRELESS CHARGING AT WITRICITY

PAGE 8

GRAPHENE PAVES THE WAY FOR NEXT-GENERATION PLASMONICS

Simulation tools bring the complex physics of two-dimensional materials and plasmonics together in a way that could change the face of optoelectronic devices.

By **DEXTER JOHNSON**

EVER SINCE A SINGLE-ATOM-THICK FILM of graphite was first successfully synthesized back in 2004 and called graphene, it has been on a decade-long ride through applications ranging from photovoltaics and next-generation batteries to electronics.

While graphene's list of desirable properties—like its electrical and thermal conductivity—initially made it attractive for electronics, its equally attractive optoelectronic capabilities were initially overlooked. But it soon became clear that graphene has incredible potential as a transparent conducting electrode and could be an alternative to the commonly used indium tin oxide (ITO). Graphene offers comparable or better optoelectronic performance in addition to its mechanical strength and flexibility. Other potential uses are diverse and include applications such as transparent conductors used in touchscreens and photovoltaics (see Figure 1), lab-on-chip devices for the sensing of viruses or proteins, improved night vision, mid-IR imaging applications, and solar cells.

FIGURE 1: Bendable and lighter smartphone and laptop screens are just one of the many applications of graphene. Others include energy, computing, engineering, and health technologies and devices.

» GRAPHENE AND PLASMONICS MEET

IN ADDITION TO OPTOELECTRONICS, graphene's star has shone particularly bright in photonics when it is used in combination with the field of plasmonics, a subfield of photonics that grew out of the need to continually explore properties and applications of light on ever-smaller scales.

Traditionally, photonics has dealt with structures on the micrometer scale, but squeezing light into smaller dimensions is fundamentally challenging due to a property of light known as the diffraction limit. Plasmonics helps with addressing this challenge and enables light confinement even at the nanoscale.

This is achieved by coupling incident light into oscillations of electrons known as plasmons—hence the name plasmonics. Today, plasmonics is an important, actively developing branch of photonics that deals with the efficient excitation, control, and use of plasmons.

» GRAPHENE-ENABLED PLASMONICS IS LEADING TO PRACTICAL DEVICES

COMPUTATIONAL NANOPHOTONICS efforts at Birck Nanotechnology Center, Purdue University, led by Alexander V. Kildishev, associate professor of electrical and computer engineering, have been leading the way in combining graphene with plasmonics to bring it closer to practical optoelectronic applications.

The work of Kildishev and his colleagues deals with a fundamental problem in graphene research: it is currently difficult to fabricate high quality, large-area graphene films. Until graphene production improves, Kildishev and his team are leveraging simulation tools to perform design and optimization of devices made from graphene.

Through both simulation and experimental testing, Kildishev and his colleagues have been able to dem-

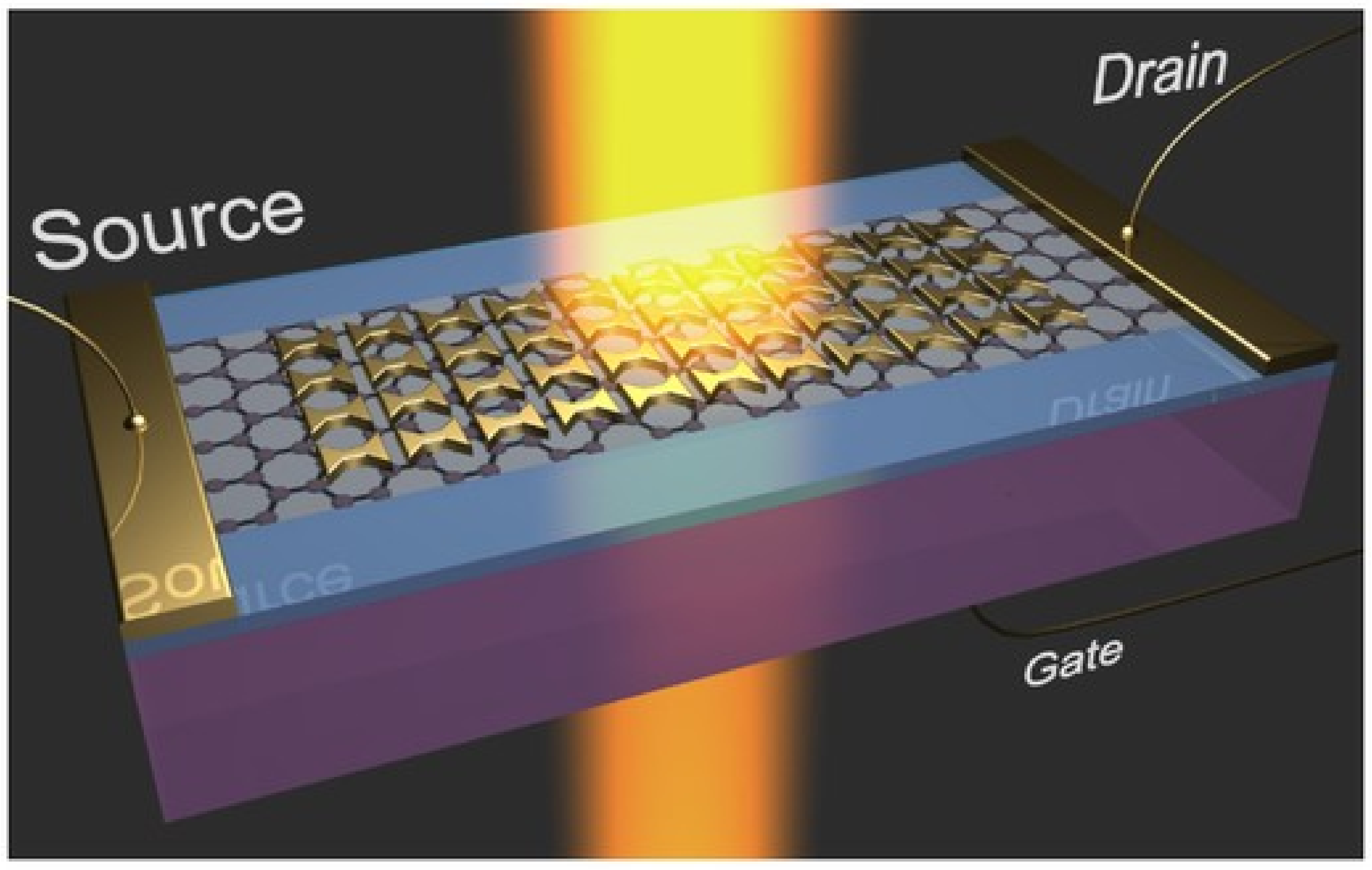


FIGURE 2: Design of Fano resonant plasmonic antennas on top of a single-layer graphene sheet optimized with COMSOL® software and its Wave Optics Module to achieve resonance at a 2 μm wavelength. The design tunability has been successfully validated in experiments using ion-gel top electrolyte gating[2].

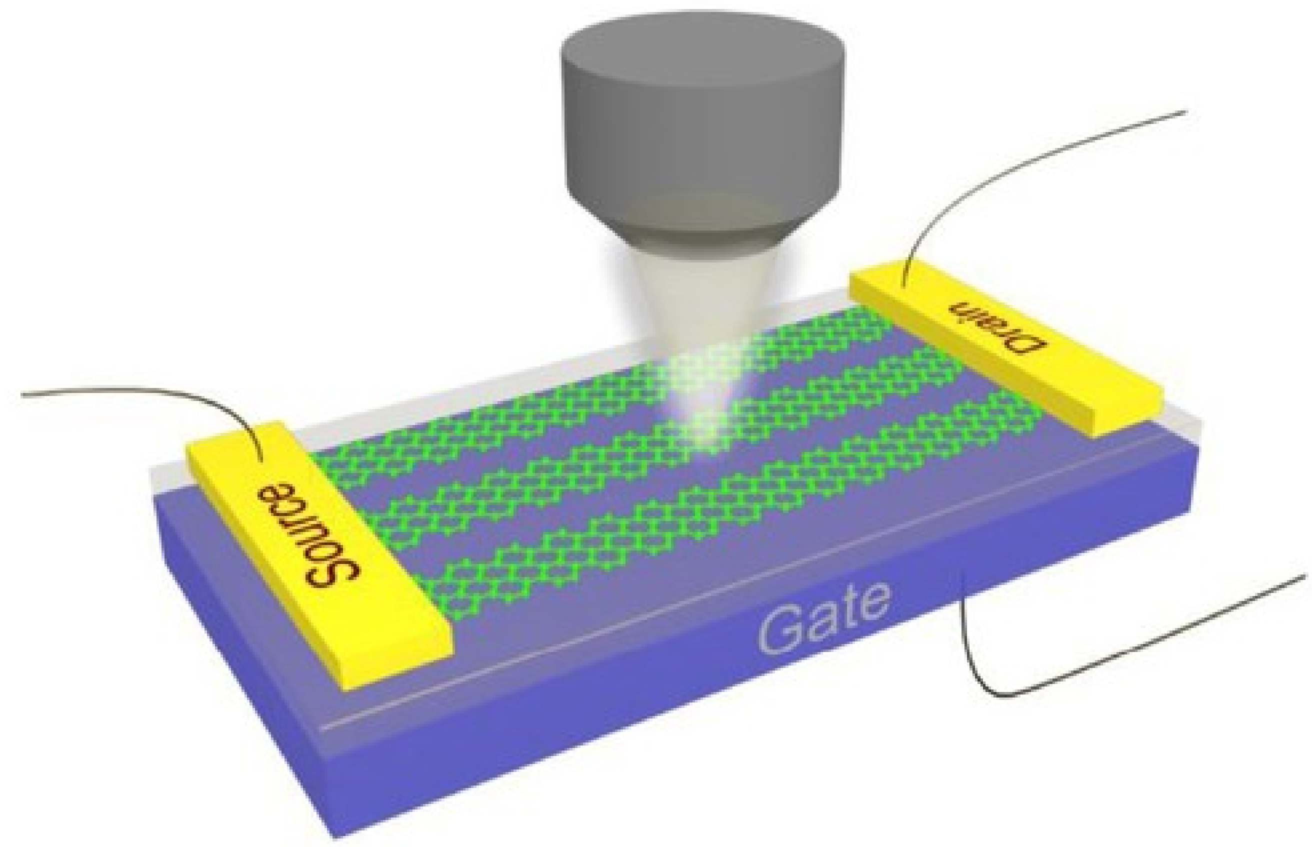


FIGURE 3: 3D artistic sketch of the experimental setup used for studying plasmon resonance in graphene nanoribbons (GNRs), simulated with COMSOL Multiphysics® software using the surface current approach. The lattice orientation of GNRs is for illustration only and dimensions are not to scale.

onstrate tunable graphene-assisted damping of plasmon resonances in nanoantenna arrays, which is important for designing tunable photonic devices in the mid-infrared range[1]. Since the mid-infrared is where fundamental vibrational resonances reside for a wide range of molecules, it is critical to have tunable plasmonic devices that work in that range for applications in sensing and imaging.

On the other hand, moving closer to even shorter infrared (IR) waves, e.g., the telecom range, is also of ultimate importance for telecommunications and optical processing. The group at Purdue has shown efficient dynamic control of Fano resonances in hybrid graphene-metal plasmonic structures at near-infrared wavelengths. Fano resonances are seen in the transmission of specifically coupled resonant optical systems. Researchers are currently leveraging the properties of Fano resonances for use in optical filtering, sensing, and modulators (see Figure 2).

Leveraging the predictive power of COMSOL Multiphysics® software models is a vital step for designing tunable elements for the next generation of plasmonic and hybrid nanophotonic on-chip devices such as sensors and photodetectors, according to Kildishev. The photodetectors could ultimately find use in the sensing of infrared electromagnetic radiation for multicolor night vision and thermal imaging. Another application may be in biosensing, where the resonant lines of plasmonic elements are tuned to match the resonances of the spectral optical responses of viruses or proteins.

In their work, the Purdue researchers combined the unique properties of graphene with plasmonic nanoantennas to modulate the antenna's optical properties. Having a tunable resonant element along an optical path is as critical to optoelectronics as having a transistor in an electric circuit.

"By using the nanopatterned graphene with an electrical gating (see Figure 3), it's possible to modulate light flow in space with unparalleled spatial resolution," said Dr. Naresh Emani, a former Ph.D. student advised by Kildishev, now with DSI, Singapore. "The reduced dimensionality and semimetallic behavior of graphene plasmonic elements gives us, along with its other properties, a very vital feature—electrical tunability. This critical functionality is not attainable with conventional metal plasmonics."

Plasmonic devices based on noble metals lack this level of control over electrical tunability. Noble metals possess a large number of electrons in the conduction band, and consequently the electrical conductivity of metals cannot be easily modulated. But since graphene is a tunable semimetal, it does not contain any electrons in the conduction band in its pristine state. Therefore, its electron concentration—and hence its electrical conductivity—can be tuned chemically, modulated electrically, or even modulated optically.

» *THE ROLE OF SIMULATION AND MODELING*

NUMERICAL MODELING has been a critical tool for the researchers, allowing them to optimize their designs without complications and the significant cost of nanofabrication processes.

"Compared to experimental work, mathematical modeling is low-cost, has the opportunity to validate its output through a reduced number of prototypes, has predictive power, and, finally, allows you to optimize for a desired functionality," explained Kildishev.

In a field where the quality of the graphene material can vary, it is critical that there always be a tight connection between numerical results and experiments in order to better understand the impact of all variables involved.

"In most cases, by fitting model

> **“** Another strength of COMSOL is its ability to model two-dimensional materials natively in terms of surface current.”
>
> —**LUDMILA PROKOPEVA, HIGH-PERFORMANCE COMPUTING SPECIALIST, BIRCK NANOTECHNOLOGY CENTER**

rations to explore the plasmonic properties of graphene in the quantum optics regime. Kildishev and his colleagues believe the quantum optics regime will be the next frontier for the science of light and has been relatively unexplored in the mid-IR wavelengths.

“Semiconductor quantum wells show some interesting quantum properties but are restricted to low temperatures so far,” said Kildishev. “If we successfully address some of the challenges in graphene research, it might end up outperforming semiconductor quantum wells. If we are able to do this, we could significantly reduce the size of many devices.” They continue to move forward on the cutting edge of research with many unknowns, toward a future that contains unbelievable possibilities. ◎

Alexander V. Kildishev, associate professor at Purdue’s Birck Nanotechnology Center.

References

[1] N. K. Emani et al., *Nano Lett.* 12, 5202–5206 (2012).

[2] N. K. Emani et al., *Nano Lett.* 14, 78–82 (2014).

[3] D. Wang et al., “Plasmon Resonance in Single- and Double-layer CVD Graphene Nanoribbons,” in CLEO: 2015, p. FTu1E.3.

[4] L. Prokopeva and A. V. Kildishev, “Time Domain Modeling of Tunable Graphene-Based Pulse-Shaping Device (invited),” in ACES 2014.

SIMULATING GRAPHENE

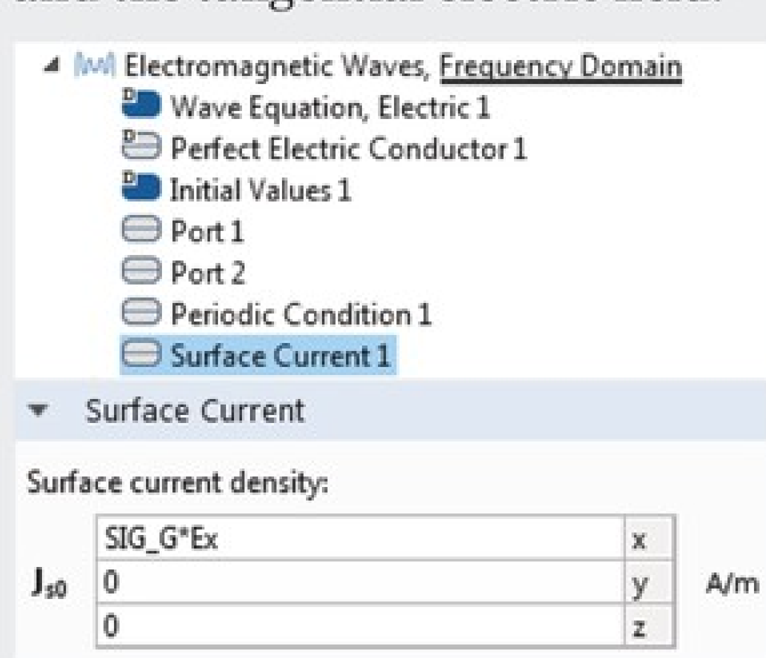
BY ANDREW STRIKWERDA

WHAT IS THE BEST WAY to simulate graphene? More specifically, should graphene actually be modeled as a 2D layer or rather as a 3D material that is extremely thin? Many researchers have used the latter approach because it is the only one supported in their numerical software. With COMSOL Multiphysics® software, you can use either method. As stated in the article, Professor Kildishev and his colleagues have found that simulating graphene as a 2D material yields better agreement with experimental results. Let’s take a closer look at how this is implemented in COMSOL® software.

Ohm’s law states that, in the frequency domain, the current density is simply the product of the conductivity and the electric field:

$$J = \sigma E$$

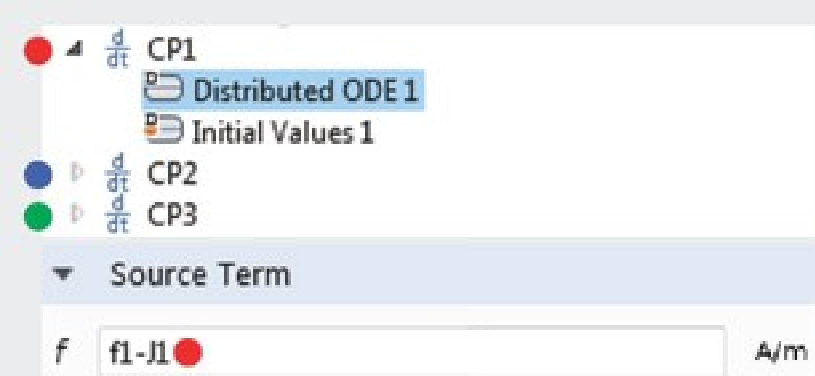
In COMSOL Multiphysics, this can be implemented in 2D using a Surface Current boundary condition where the induced current is expressed, according to Ohm’s law, as the product of the graphene conductivity (calculated, for example, from a Random Phase Approximation) and the tangential electric field.



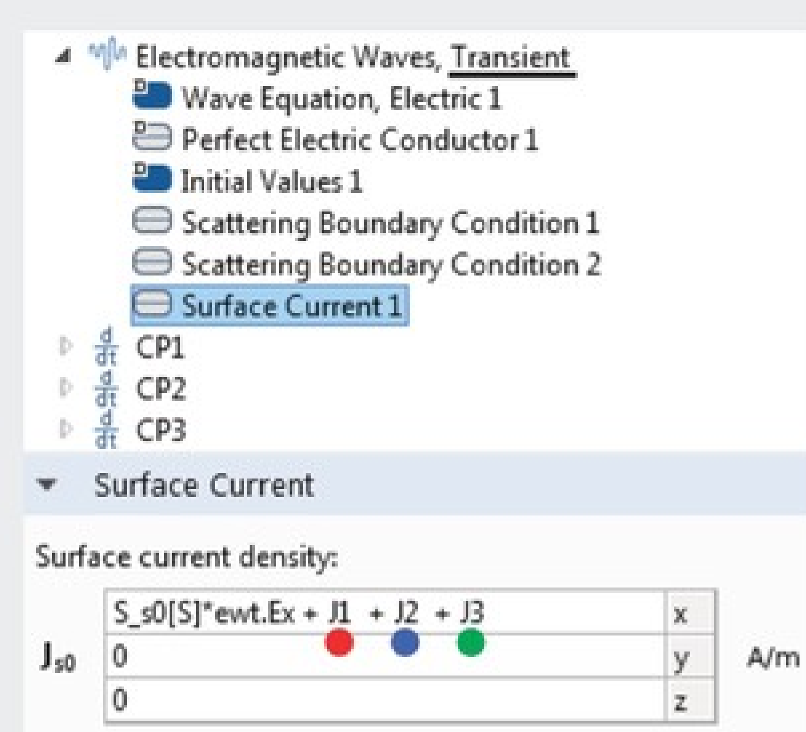
For time-domain simulations, the required surface current density can be a little more difficult to calculate, since Ohm’s law is now a convolution of the electric field and the conductivity:

$$J(t) = \int_{-\infty}^{t} \sigma(t-\tau)E(\tau)d\tau$$

To implement this in COMSOL (see Figure 4), Professor Kildishev’s group used a Padé approximation to represent the frequency-dependent optical conductivity of graphene. They then applied a Fourier transform of the terms in the Padé series to obtain second order partial differential equations in time, which can be solved in COMSOL.



The solutions to these equations, representing contributions to the time-dependent surface current, can then be linked to the Surface Current boundary condition.



If you would like to learn more about how to simulate graphene, watch the webinar by Alexander Kildishev on comsol.com/webinars and download his COMSOL models available at comsol.com/community/exchange/361.