

A Self-Consistent Wave-Optics Workflow for Graphene Nonlinearity in a D-Shaped Fiber

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Abstract

Graphene-coated optical fibers are a promising platform for nonlinear modulation, but they are computationally demanding to model. Graphene conductivity depends nonlinearly on the local optical field, while the sheet itself is atomically thin within a fiber-scale cross-section. We present a self-consistent COMSOL Multiphysics®–MATLAB® framework that combines a two-dimensional linear eigenmode calculation with iterative updates of the intensity-dependent graphene surface conductivity. Two independently coded nonlinear pathways agree closely and converge within three iterations over the reported range. The model predicts coupled changes in modal effective index and attenuation for efficient design space exploration.

Keywords: Graphene; Nonlinear optics; D-shaped fiber; Surface conductivity; Self-consistent modeling.

1. Introduction

Graphene-coated optical fibers are an attractive platform for all-fiber optical switching and modulation. Graphene combines an electrically tunable optical conductivity with a strong nonlinear optical response, enabling the guided optical field to be modified through changes in its material state. A side-polished D-shaped fiber provides evanescent-field access to graphene near the guided core mode while retaining much of the original fiber structure and compatibility with standard fiber processing [1]. The structure considered in this work is shown in Fig. 1(a). Rather than using a single graphene layer, a graphene–dielectric–graphene stack forms a dual-graphene capacitor in which an applied differential bias induces equal and opposite carrier densities in the two graphene sheets. Because both sheets interact with the guided optical field, the resulting changes in their optical conductivities contribute jointly to the modal response, providing efficient electrostatic control of the device operating point [2]. The optical response depends jointly on several design and operating parameters—including the residual cladding thickness above the core, dielectric thickness, applied bias and optical power—making numerical modeling invaluable for understanding the device behavior and exploring the design space prior to fabrication.

Modeling this structure at optical frequencies is numerically demanding without an appropriate reduction strategy. The atomically thin graphene sheets sit within a fiber cross-section several orders of magnitude larger, so resolving their thickness explicitly requires extreme local mesh refinement across highly disparate length scales. Extending such a mesh over a device-scale propagation length in three dimensions can result in runtimes of days,

making repeated simulations impractical for design screening. In COMSOL Multiphysics®, graphene can instead be represented using the Transition Boundary Condition (TBC), which captures the sheet response through an equivalent surface conductivity without explicitly meshing its thickness [3]. Although this removes the principal subwavelength meshing burden, three-dimensional (3D) simulations with intensity-dependent material properties remain computationally expensive. A two-dimensional (2D) eigenmode analysis is far more efficient but, for a fixed material state, is linear and therefore cannot directly determine a graphene conductivity that depends on the local intensity it produces. The challenge is thus to retain the efficiency of the 2D eigenmode calculation while closing the feedback loop between the solved optical field and the intensity-dependent graphene material state.

Our methodology is therefore to retain COMSOL's efficient 2D linear eigenmode solve while handling the intensity-dependent graphene response externally through LiveLink™ for MATLAB®. COMSOL solves the eigenmode problem for a fixed graphene material state; MATLAB extracts the graphene-surface intensity and effective modal index, evaluates the corresponding nonlinear update to the surface conductivity, and returns it to the TBC; and the cycle repeats until the complex effective index converges. Each nonlinear operating point is therefore obtained through a converged sequence of linear eigenmode solutions.

2. Physical Model and Self-Consistent COMSOL-MATLAB Framework

2.1 Device and Optical Model

The model geometry is the transverse cross-section of the graphene-coated D-shaped fiber shown in Fig. 1(a). A standard silica fiber of core radius $4.1\ \mu\text{m}$ is side-polished to leave a residual cladding thickness ($t_{\text{remain}} = 0.1\ \mu\text{m}$) above the core. A graphene- Ta_2O_5 -graphene stack is deposited on the polished flat, with a dielectric thickness $t_{\text{dielectric}} = 100\ \text{nm}$ separating the two graphene sheets. The optical model is evaluated at a wavelength, $\lambda = 1.53\ \mu\text{m}$.

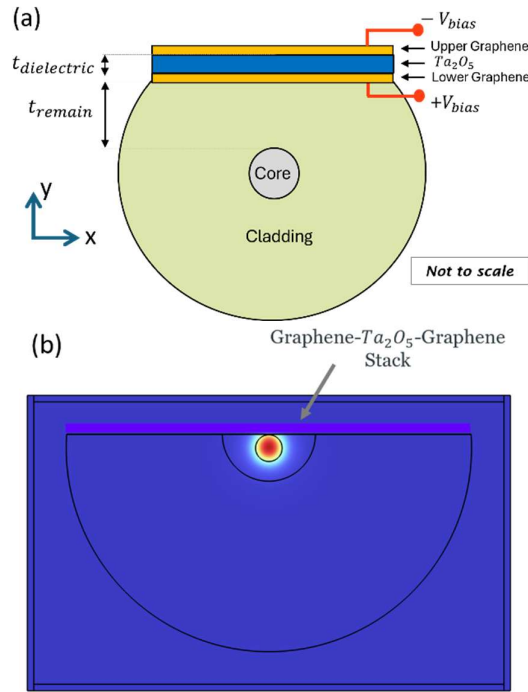


Figure 1. Graphene-coated D-shaped fiber geometry and guided mode: (a) cross-sectional device schematic; (b) representative x-polarized core-guided mode profile.

The guided mode is calculated using a 2D Mode Analysis study within the Electromagnetic Waves, Frequency Domain interface of COMSOL Multiphysics® version 6.4 using the Wave Optics Module. Side polishing breaks the cylindrical symmetry of the fiber and separates the two orthogonal polarization branches. The x-polarization branch is used throughout this work as its interaction with the graphene-coated flat is substantially stronger than that of the orthogonal y-polarization mode while remaining predominantly core guided. To quantify this interaction, we use the coefficient $P_{\text{g,tangential}}/P_{\text{mode}}$, where $P_{\text{g,tangential}}$ is the tangential-field-weighted power per unit length obtained by integrating $|E_t|^2$ along the graphene boundary and P_{mode} is the total guided modal power.

For the geometry considered here, this coefficient is approximately 67 times greater for the x-polarization than for the y-polarization. A representative field profile is shown in Fig. 1(b).

Each graphene monolayer is approximated using the COMSOL TBC, with its optical response specified through a complex surface conductivity. This thin-layer treatment avoids explicitly resolving the 0.335 nm graphene thickness in the finite-element mesh while retaining its electromagnetic influence on the guided mode. For a specified conductivity on each graphene boundary, COMSOL solves a linear eigenmode problem and returns the complex modal effective index (n_{eff}) together with the field quantities at the graphene surfaces required for the subsequent material-response calculation. The intensity dependence of that material response, and its coupling back to the eigenmode solution, are introduced in the following subsections.

2.2 Graphene Linear and Nonlinear Material Response

The graphene material relations below are evaluated separately for the upper and lower sheets (sheet labels are omitted for clarity).

Because graphene is a 2D material, its optical response is naturally described by a complex surface conductivity. In the linear regime, the conductivity is calculated using the finite-temperature Kubo formulation [4],

$$\sigma_{\text{Kubo}}(\omega, E_F) = \sigma_{\text{intra}}(\omega, E_F) + \sigma_{\text{inter}}(\omega, E_F),$$

where E_F is the graphene Fermi level and $\omega = 2\pi c/\lambda$ is the angular optical frequency, with c the speed of light. For a given Fermi level, the Kubo formulation defines the linear surface conductivity; the dependence of the Fermi level on electrical bias is described in Section 2.3. Both intraband and interband contributions are considered, with $T = 300\ \text{K}$ and a carrier-scattering relaxation time $\tau = 0.1\ \text{ps}$.

To incorporate nonlinear effects, we use the conventional perturbative expansion of the optical polarization, truncated after the third-order contribution [5]:

$$\mathbf{P}(\omega) = \epsilon_0 [\chi^{(1)} \mathbf{E} + \chi^{(3)} |\mathbf{E}|^2 \mathbf{E}],$$

where ϵ_0 is the vacuum permittivity, $\mathbf{E}$ is the electric-field phasor, and $\chi^{(1)}$ and $\chi^{(3)}$ denote the effective linear and third-order susceptibilities. The third-order polarization produces an intensity-dependent modification of graphene's complex optical response relative to the linear Kubo state. This modification may be represented either through an equivalent complex refractive index or, equivalently, through a change in the surface conductivity supplied to the COMSOL TBC. We therefore implement the same nonlinear material response

using two formulations: an index-based n_{NL} pathway and a conductivity-based σ_{NL} pathway. A small Kerr correction to the Ta_2O_5 spacer is also included in the material update.

The two formulations are related through the complex graphene index $\tilde{n} = n - ik$ (using COMSOL's $e^{i\omega t}$ phasor convention) where n is the refractive index and k the extinction coefficient. The complex index is related to the surface conductivity by

$$\sigma = i\epsilon_0\omega d_{\text{eff}}(\tilde{n}^2 - n_{\text{host}}^2),$$

where $d_{\text{eff}} = 0.335 \text{ nm}$ is the effective graphene thickness and n_{host} is the effective background index obtained from the mean permittivity of the media adjoining each graphene sheet ($n_{\text{host}} = 1.772$ and 1.610 for the lower and upper sheets, respectively). The Kubo conductivity can therefore be represented by an equivalent complex index $\tilde{n}_{\text{Kubo}}$.

In the n_{NL} formulation, the third-order correction is incorporated using the index mapping [6],

$$\tilde{n}_{NL} = \sqrt{\tilde{n}_{\text{Kubo}}^2 + 2\tilde{n}_{\text{Kubo}}\Delta\tilde{n}}.$$

For $|\Delta\tilde{n}| \ll |\tilde{n}_{\text{Kubo}}|$, this reduces to the familiar small-perturbation form $\tilde{n}_{NL} \approx \tilde{n}_{\text{Kubo}} + \Delta\tilde{n}$. Alternatively, the same third-order response is represented directly in conductivity space as

$$\sigma_{NL} = \sigma_{\text{Kubo}} + \Delta\sigma_{NL},$$

$$\Delta\sigma_{NL} = i\epsilon_0\omega d_{\text{eff}}(2\tilde{n}_{\text{Kubo}}\Delta\tilde{n}).$$

The two formulations are algebraically equivalent but were implemented independently to provide an internal cross-check of the complex index-conductivity mapping and its implementation within the self-consistent framework. In both cases, the final material quantity supplied to the COMSOL TBC is the nonlinear surface conductivity σ_{NL} .

For both formulations, the complex nonlinear correction combines refractive and absorptive effects,

$$\Delta\tilde{n} = \Delta n - i\Delta k = \frac{(n_2 - ik_2)I_g}{1 + I_g/I_{\text{sat}}},$$

where I_g is the intensity-weighted effective tangential optical intensity along the graphene sheet. The nonlinear coefficients n_2 and k_2 are obtained from the small-signal values in Ooi *et al.* [4], after conversion from their bulk-intensity convention to the graphene sheet-intensity convention used here. The converted coefficients are updated as the graphene material state evolves during the self-consistent iteration. The denominator introduces phenomenological saturation [4,5], with $I_{\text{sat}} = -mk_0/k_2$, where k_0 is the extinction coefficient of the initial Kubo state and $m = 0.8$ the saturable fraction. A lower bound $k \geq (1 - m)k_0$ is retained

to represent the nonsaturable extinction component and is applied only if the nonlinear update would otherwise fall below this value. This constraint is inactive over the reported range. I_{sat} is established from the initial Kubo state for each operating point and held fixed during the subsequent self-consistent iteration.

2.3 Bias-Dependent Kubo State

The Kubo baseline used in the nonlinear calculation is established by the electrically induced carrier density in the graphene- Ta_2O_5 -graphene capacitor. A differential voltage V_{diff} is imposed across the graphene stack, producing equal and opposite static carrier densities in the two sheets [2]. Using the analytical parallel-plate approximation, with graphene quantum-capacitance corrections neglected, the magnitude of the bias-induced carrier density is

$$n_{0,V} = \frac{\epsilon_0\epsilon_r}{e\epsilon_{\text{dielectric}}}V_{\text{diff}},$$

where $\epsilon_r = 25$ is the low-frequency relative permittivity of Ta_2O_5 and e is the elementary charge. The calculations presented here use $V_{\text{diff}} = 1.2 \text{ V}$. The validity of this electrostatic approximation for the present geometry is examined independently in Section 3.3.

The graphene sheets are therefore assigned equal-magnitude, opposite signed equilibrium carrier densities, $n = \pm n_{0,V}$.

The corresponding Fermi level is obtained from graphene's linear dispersion relation [7],

$$E_F = \hbar v_F \sqrt{\pi|n|} \text{sgn}(n),$$

where $v_F = 1 \times 10^6 \text{ m s}^{-1}$ is the graphene Fermi velocity. This bias-set Fermi level defines the equilibrium Kubo conductivity $\sigma_{\text{Kubo}}(\omega, E_F)$ for each graphene sheet. Photoexcited nonequilibrium carrier populations are not modeled explicitly. Instead, the intensity-dependent optical response is represented through the phenomenological complex third-order correction $\Delta\tilde{n}(I)$ introduced in Section 2.2.

2.4 Self-Consistent Iteration

For each prescribed input power P_{in} , the calculation begins with a Kubo-only eigenmode solution. The eigenmode returned by COMSOL has an arbitrary amplitude. Its calculated guided modal power P_{mode} is therefore used to scale the $|E|^2$ -based quantities by $P_{\text{in}}/P_{\text{mode}}$, thereby normalizing the solution to the prescribed launched peak power. The graphene intensity I_g is evaluated at each graphene sheet and passed to MATLAB® through LiveLink™, where the intensity-dependent complex nonlinear correction $\Delta\tilde{n}$ is calculated. Either the n_{NL} or σ_{NL}

pathway described in Section 2.2 is then used to obtain an updated surface conductivity σ_{NL} . This conductivity is returned to the COMSOL TBC and the eigenmode problem is solved again using the updated graphene material state. The process is repeated until the relative change in the complex modal effective index satisfies

$$\epsilon_k = \frac{|n_{\text{eff}}^{(k)} - n_{\text{eff}}^{(k-1)}|}{|n_{\text{eff}}^{(k-1)}|} < \epsilon_{\text{tol}},$$

where ϵ_k is the relative effective-index change between successive iterations.

At convergence, the graphene material state supplied to COMSOL is consistent, as assessed by the effective index convergence criterion, with the modal field produced by that material state. Each nonlinear operating point is therefore obtained as a self-consistent sequence of linear 2D eigenmode solutions [8] rather than through a directly coupled nonlinear field solution. This separation retains the computational efficiency of the linear COMSOL eigen solver while preserving the feedback between the optical mode and the intensity-dependent graphene response. For this study, a longitudinal segment length of 250 μm is used, over which the graphene material state is treated as locally uniform. Longer devices can be represented by cascading such segments, with the output optical power from one segment used as the input to the next. The complete computational workflow is summarized in Fig. 2.

3. Model Verification and Convergence

The framework was assessed through three complementary checks: pathway equivalence, numerical convergence, and an electrostatic test of the static-gating approximation.

3.1 Equivalence of the Nonlinear Material-Update Pathways

The n_{NL} and σ_{NL} pathways are algebraically equivalent but were coded independently to verify the complex index-conductivity mapping and nonlinear update within the complete solver. Because both ultimately supply the graphene TBC with the nonlinear surface conductivity, agreement in the converged conductivity directly tests whether the independent implementations produce the same material state. This is therefore an implementation check rather than an independent validation of graphene physics.

Fig. 3(a) shows essentially indistinguishable values of $|\sigma_{NL}|$ through $I_g/I_{\text{sat}} \approx 2.5$, with corresponding phase agreement across the reported range (not shown), confirming that the two separate implementations apply the complex index-conductivity mapping consistently.

3.2 Numerical Convergence

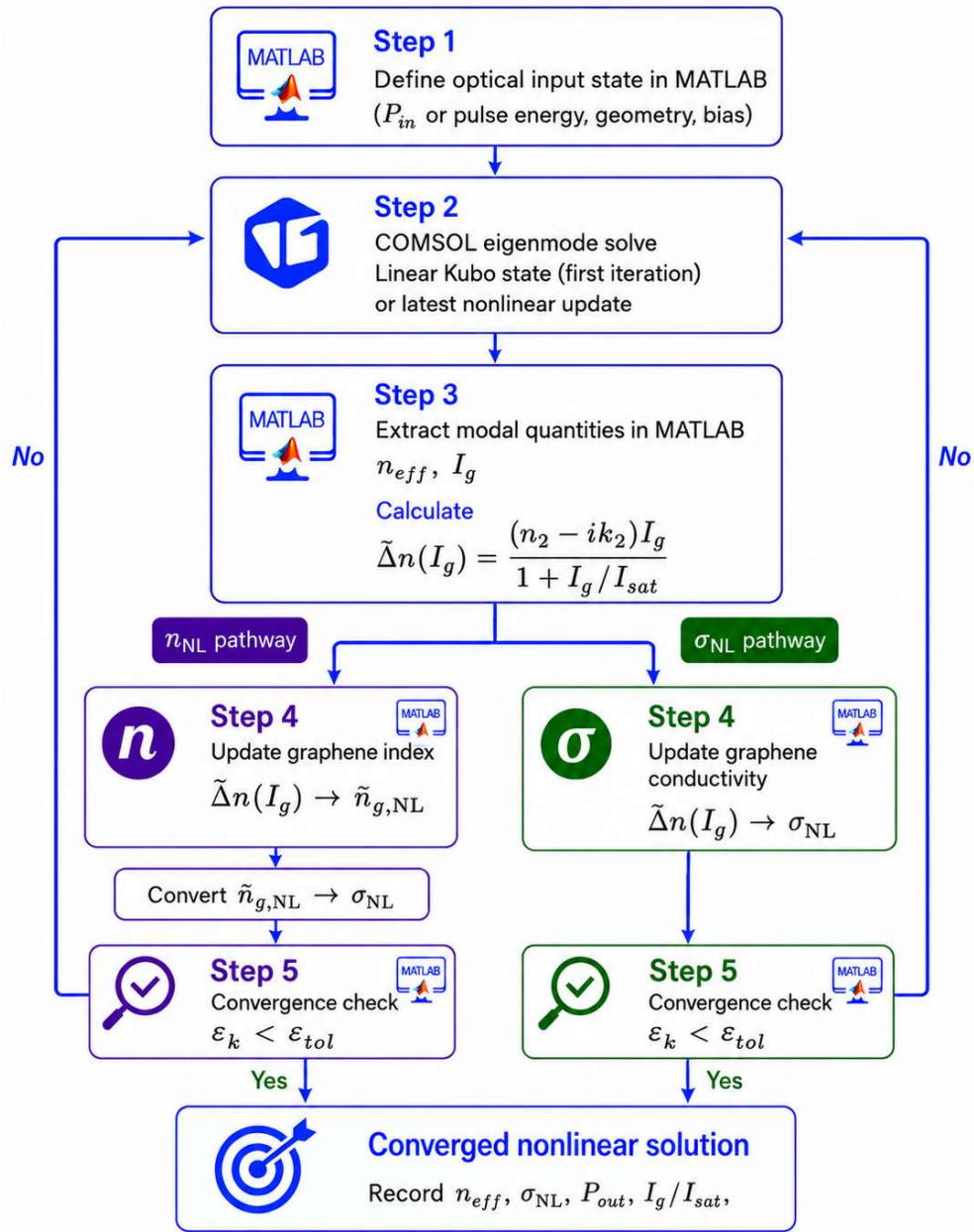
The convergence of the self-consistent COMSOL–MATLAB loop was assessed using the relative effective-index change defined in Section 2.4. Fig. 3(b) shows the normalized convergence measure $\epsilon_k/\epsilon_{\text{tol}}$ for representative low-, intermediate- and high-intensity operating points, with convergence reached when this quantity falls below unity. A convergence tolerance of $\epsilon_{\text{tol}} = 5 \times 10^{-6}$ was used throughout the reported simulations.

Across the seven operating points used in the reported nonlinear sweep, convergence was achieved within three iterations. The corresponding iteration counts were between one and three, with the higher-intensity cases generally requiring the additional update. Fig. 3(b) illustrates this progression using representative cases near $I_g/I_{\text{sat}} \approx 0.10, 1.00$, and 2.50 . Additional calculations (not shown) using a tighter convergence tolerance were performed to test whether the chosen tolerance materially affected the converged solution. Tightening the convergence tolerance from 5×10^{-6} to 10^{-8} produced maximum absolute differences of less than 2×10^{-8} in $\text{Re}(n_{\text{eff}})$ and 1×10^{-6} in the modal overlap over the reported excitation range. The 5×10^{-6} criterion was therefore retained as an appropriate compromise between convergence accuracy and computational cost for the design-trend calculations presented here. In the present implementation, a nonlinear operating point required approximately two minutes to converge.

A separate mesh-refinement check increased the number of 2D domain elements from $\sim 6.8 \times 10^4$ to $\sim 1.3 \times 10^5$. At the Kubo baseline and the highest reported nonlinear excitation, I_g and attenuation (α_{eff}) changed by less than 0.2%, while the absolute change in $\text{Re}(n_{\text{eff}})$ remained below 6×10^{-7} .

3.3 Electrostatics Check of the Parallel-Plate Approximation

The optical model described in Section 2 uses an analytical parallel-plate approximation to establish the bias-induced carrier density in the graphene– Ta_2O_5 –graphene stack. To test this assumption using an independent physical formulation, the COMSOL model was augmented with an Electrostatics (ES) physics interface, in addition to the Wave Optics physics used for the eigenmode calculations. The electrostatic calculation was performed separately rather than as a coupled optical–electrostatic multiphysics solution, allowing the analytical gating approximation to be checked directly against a finite-element solution of the actual D-shaped geometry. Using the same 100 nm Ta_2O_5 layer as in the optical model, potentials of +0.6 V and –0.6 V were applied to the lower and upper graphene sheets,



In both pathways, the final material parameter returned to COMSOL is the nonlinear graphene surface conductivity used in the Transition Boundary Condition.

Figure 2. Self-consistent COMSOL–MATLAB workflow

respectively, corresponding to $V_{\text{diff}} = 1.2 \text{ V}$. Fig. 4 shows that the electrostatic potential varies nearly linearly across the dielectric between the two graphene sheets, as expected for the parallel-plate approximation. The static carrier density obtained from the Electrostatics solution was $n_{\text{ES}} = 1.65804 \times 10^{16} \text{ m}^{-2}$, compared with $n_{\text{pp}} = 1.65790 \times 10^{16} \text{ m}^{-2}$ from the analytical expression used in the nonlinear optical model, corresponding

to a relative difference of $\sim 0.008\%$. The close agreement provides an independent physics check of the parallel-plate approximation for this geometry; quantum-capacitance effects are not included in these calculations.

4. Nonlinear Modal Response and Discussion

Fig. 5 shows the converged modal response as the lower-sheet graphene intensity increases from the

weak-excitation regime to approximately $I_g/I_{\text{sat}} = 2.5$. The n_{NL} and σ_{NL} pathways remain closely overlapping across the displayed range.

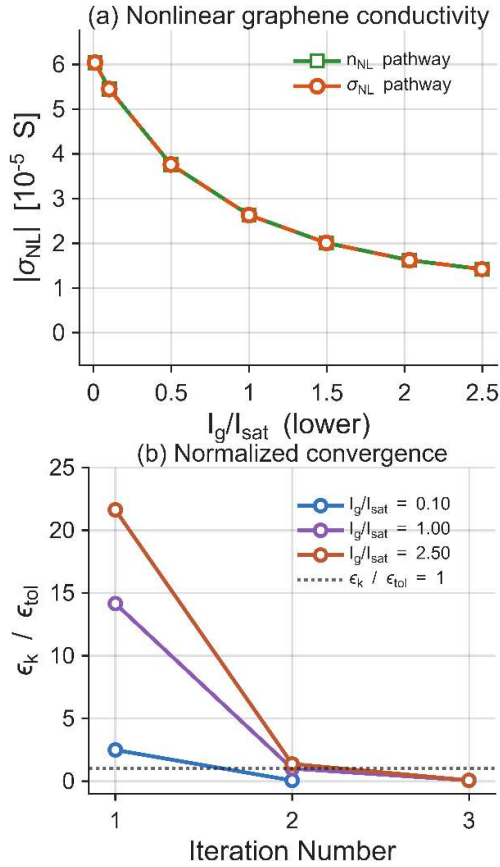


Figure 3. Model verification: (a) converged nonlinear graphene conductivity from the n_{NL} and σ_{NL} pathways; (b) normalized convergence at representative I_g/I_{sat} .

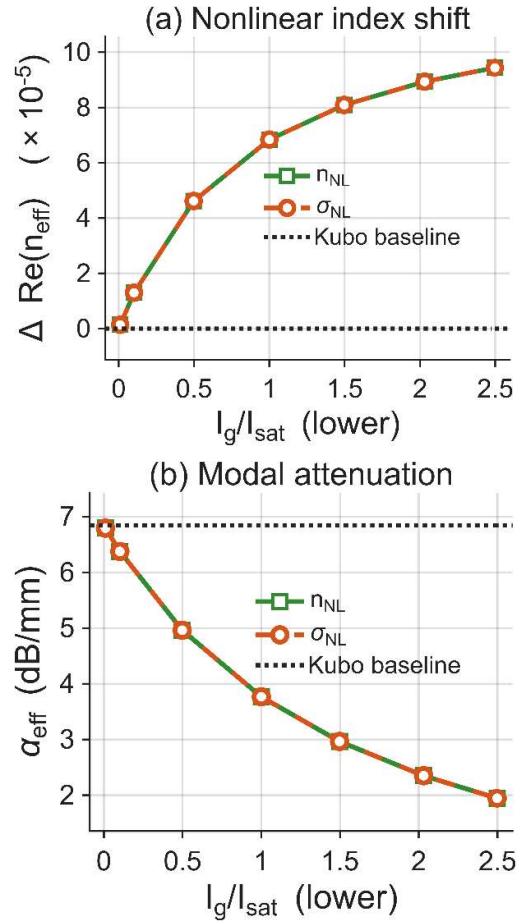


Figure 5. Converged nonlinear modal response versus lower-sheet I_g/I_{sat} : (a) nonlinear shift in $\text{Re}(n_{\text{eff}})$; (b) effective modal attenuation. The n_{NL} and σ_{NL} pathways are compared with the Kubo-only baseline.

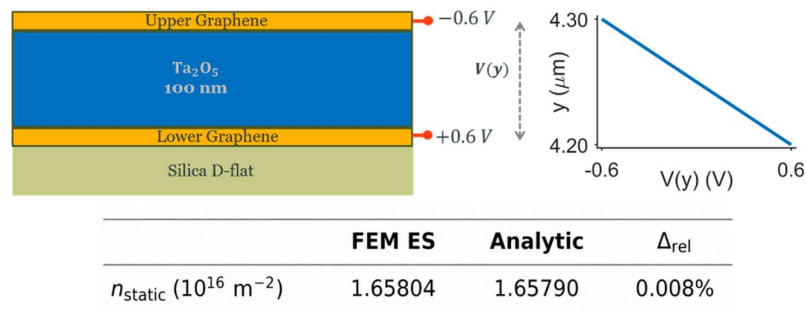


Figure 4. COMSOL Electrostatics check of the parallel-plate static-gating approximation

Relative to the Kubo-only baseline, the nonlinear shift in $\text{Re}(n_{\text{eff}})$ increases in magnitude with increasing I_g/I_{sat} and begins to saturate at higher excitation [Fig. 5(a)]. At the same time, the effective modal attenuation decreases [Fig. 5(b)], consistent with the increasing bleaching of graphene absorption [1]. These refractive and absorptive changes are not independent effects. The graphene response is complex, $\Delta\tilde{n} = \Delta n - i\Delta k$, so changes in refraction and absorption enter the same material update. The resulting complex conductivity modifies the eigenmode, which in turn changes the graphene intensity I_g . The updated I_g changes the complex nonlinear correction $\Delta\tilde{n}(I_g)$, and hence the nonlinear surface conductivity σ_{NL} supplied to the next eigenmode solve. The final modal response therefore reflects the coupled absorptive–refractive feedback of the complete self-consistent loop.

The nonlinear update does not produce any significant change in modal character over the reported range. The modal overlap of the converged nonlinear mode with the Kubo-only mode at the same operating point remains high, with a minimum modal overlap of ~ 0.9975 . This indicates that the calculations remain on the same core-guided x-polarized modal branch as the graphene material state evolves, while the complex modal effective index and attenuation change continuously with excitation.

5. Conclusions

A self-consistent COMSOL–MATLAB framework has been developed for modeling the nonlinear optical response of graphene-coated D-shaped fiber using a 2D linear eigenmode solver. Graphene is represented through a surface conductivity using COMSOL’s TBC, while the intensity-dependent nonlinear material response is evaluated externally in MATLAB and iteratively returned to COMSOL. In this way, each nonlinear operating point is obtained as a converged sequence of linear eigenmode solutions, avoiding the computational cost of a fully 3D nonlinear optical model.

The framework was verified through three complementary checks. Independently implemented n_{NL} and σ_{NL} material-update pathways produced essentially identical converged surface conductivities, the self-consistent iteration converged within three iterations over the reported range using $\epsilon_{\text{tol}} = 5 \times 10^{-6}$, and an independent COMSOL Electrostatics calculation supported the parallel-plate approximation used to establish the static graphene carrier state. Applied to the D-shaped fiber, the converged model predicts a coupled nonlinear shift in $\text{Re}(n_{\text{eff}})$ and reduction in modal attenuation with increasing graphene intensity, while

maintaining the same guided modal family across the investigated range.

The dimensions used here define a representative device geometry for demonstrating the workflow. The method is intended primarily as a computationally efficient tool for identifying nonlinear modal trends and design sensitivities rather than for predicting experimentally calibrated absolute device performance. It therefore provides a practical intermediate modeling level between a purely linear transverse-mode calculation and substantially more computationally intensive device-level simulations, and can be used to guide subsequent geometry refinement, higher-dimensional modeling and experimental design.

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