Full-Wave Nonlinear Optical Analyses of Graphene-Based Optoelectronic Devices

Jun Niu[1], Ma Luo[2], and Qing H. Liu*[1]

[1] Duke University, Durham, NC, USA

[2] Wave Computation Technologies, Durham, NC, USA

Graphene has drawn strong interest and intensive study because of its remarkable electromagnetic, thermal, and mechanical properties. As a crucial property, graphene's nonlinear optical performance is an emerging topic in theoretical and experimental studies. Recent investigations shows that despite its one-atom thickness, single layer graphene's nonlinear optical response is particularly strong. Due to the centrosymmetric structure, the ideal floating single layer graphene forbids the emission of second harmonic generation (SHG) of optical fields. However, in practical designs, the symmetric property may be broken by its adjacent materials, which makes the induced SHG optical behavior interesting. On the contrary, the third order nonlinear optical effects in graphene are reported as remarkably strong. Originated from the resonant nature of the light-graphene interaction, the effective third-order susceptibility arrives on the order of $|\chi^{(3)}| \sim 10^{-15} m^2/V^2$. This strong third order optical interaction generates a third harmonic signal with a significant contrast between graphene and the background material in most optoelectronic designs.

Current studies in graphene's nonlinear performance are mainly based on experimental measurements and analytical studies. However, both approaches have serious limitations in practical applications. Only for relatively simple structures, such as floating single layer graphene or graphene deposed on flat substrate, the analytical approach is able to effectively analysis the nonlinear optical performance of graphene, and contribute to the determination of graphene's material parameters. Meanwhile, experimental measurement may provide a persuasive result, but is usually beyond consideration for the design process of complex graphene-based optoelectronic devices.

In this work, a full-wave numerical solver is proposed for nonlinear optical analysis of graphene-based optoelectronic devices. Based on the method of boundary-integral spectral element method (BI-SEM), the optical field components at fundamental frequency (FF) and generated frequencies are solved together. BI-SEM performs a spectral accuracy, i.e. the relatively error decreases exponentially with the increase of Gauss-Lobatto-Legendre (GLL) basis functions' order. With this fast convergence method, the proposed numerical scheme is able to solve the FF field and the new generated fields accurately with a relatively high convergence rate. Meanwhile, the flexibility of spectral element method also makes this scheme suitable for the simulation of more complex optoelectronic designs.