Enhancing Scattering and Absorption in Two-Dimensional Layered Material Systems with Surface Plasmons and Periodicity

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***Abstract* —** The electromagnetic waves scattered or absorbed by the structures having atomically thin layered materials can be enhanced by surface plasmon resonance and periodicity. In this work, we show that the enhancement can be accurately calculated using analytical methods specifically developed for multilayered media. Analytical methods' accuracy and efficiency is compared against experimental results found in the literature and commercially available full wave electromagnetic solvers, respectively.

***Index Terms* –** Coupled dipole approximation, field enhancement, graphene, surface plasmon resonance, two-dimensional layered materials.

I. INTRODUCTION

Graphene, the vanguard of two-dimensional (2D) materials, has proven that the atomically thin layered materials have unprecedented electrical, optical, and mechanical properties and they will play a crucial role in future opto-electronic technologies [1]. Recent studies [2] show that excitons in 2D transition metal dichalcogenides (TMDs) have a radius and a binding energy values between those values for Frenkel and Wannier-Mott excitons. Since their band gap energy falls in the visible part of the electromagnetic (EM) spectrum, they can easily be utilized in optical and opto-electronic devices. Unlike the excitons creating the light emission in semiconductors at low temperatures, excitons in TMDs are observable and active even at room temperature.

It is known that the scattered field from a 2D material coated substrate can be enhanced by decorating its surface with metal nano-particles. On the other hand, finite 1D periodic structures, where semiconducting thin films and lossless dielectric layers are stacked together, show an enhanced broadband absorption compared to bulk semiconductors. In this work, we first estimate the enhancement ratios in these two different structures using analytical approximate methods. Second, we compare the accuracy and efficiency of these methods against full wave EM solvers for reproducing the experimental results found in the literature.

II. THEORY

A. Modeling of 2D layered materials

2D materials can be defined either as an infinitely thin material with an optical conductivity or as a thin layer with a finite thickness and an effective complex electrical permittivity. In our early work [3], we calculate layered medium Green's functions according to these two definitions for multilayered structures including 2D materials. It is found that numerical methods show a good agreement especially in the far field. However, the latter requires significantly less computation time than the former. This is why we define atomically thin 2D materials with a finite thickness and complex electrical permittivity. Temperature and Fermi level dependent TMD model will be discussed at the conference; see [4] and [5] for graphene and MoS_2, respectively.

B. Coupled dipole approximation (CDA)

In order to estimate the enhancement in the electric field scattered from a metal nano-particle decorated substrate, we utilize the coupled dipole approximation [5]. The polarizability of molecules and metal particles are calculated taking the material composition, particle size and shape, and inhomogeneous background into account. For the optical constants of metals, experimental values are used rather than the Drude model to eliminate any concern regarding the selection of appropriate values for plasmon and relaxation frequencies.

C. Transfer-matrix method

In order to estimate the enhancement in the absorption of the electric field by a 1D periodic structure, we utilize the transfer-matrix method. We first calculate the absorption for a structure, where N, the number of units, is very large ($\sim 10^4$) to find the optimum dielectric layer thickness. Then we calculate the absorption as a function of N to find the smallest N value satisfying the required absorption level.

III. APPLICATIONS

A. Surface enhanced Raman scattering (SERS)

In order to mimic the SERS examples found in the literature (i.e. [6]) where researchers utilize metal nanoparticle arrays on graphene or thin TMD coated substrates, we use the CDA by assuming the same physical properties implemented in the experiments. Numerical results, which will be discussed in detail at the conference, show that the CDA is capable of estimating the general trend in the field enhancement ratio as a function of wavelength, however it overestimates the enhancement ratios by 10-12 %. On the other hand, commercially available software packages (i.e., Lumerical and Wavenology) can reproduce experimental results with errors less than 1% but they require much longer computation times and much larger memories to analyze these multi-scale systems, where atomically thin materials coexist with orders-of-magnitude larger structures. As a result, we suggest using CDA-like fast analytical methods to determine array properties to have the maximum possible field enhancement at the desired wavelength and using a full wave equation solver to obtain an very accurate estimation of the enhancement ratio.

B. TMD based periodic structures as ultra-wideband absorbers

Even though 1D periodic multilayer stacks are much thicker than plasmonic and metamaterial absorbers, still they can be the key for broadband absorption. In this work, we theoretically examine the possibility of using mono and a few layers of TMDs in a finite length, 1D periodic structure as an ultra-wideband absorber.

The bandwidth of such structures can be expanded by changing the thickness of the dielectric layer and the number of TMD layers. Our optimum design yields broadband and nearly polarization-independent light absorption over the entire visible spectrum (350-700 nm) with an average absorption of 94.7 %. Compared to plasmonic and metamaterial-based absorbers, this is an unprecedented performance considering the amount of ohmic losses in metals.

IV. CONCLUSION

To sum up, analytical methods are still very useful to design optical and opto-electronic devices where electromagnetic waves interact with atomically thin layered materials and sub-wavelength metallic structures. At the conference, advantages and disadvantages of aforementioned analytical methods will be discussed and some new rule of thumbs will be introduced for the successful analysis and design of 2D layered material systems.

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