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High–Order Spectral Simulation of Dispersive Two–Dimensional Materials

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Abstract. Over the past twenty years, the field of plasmonics has been revolutionized with the isolation and utilization of two–dimensional materials, particularly graphene. Consequently, there is significant interest in rapid, robust, and highly accurate computational schemes which can incorporate such materials. Standard volumetric approaches can be contemplated, but these require huge computational resources. Here we describe an algorithm which addresses this issue for nonlocal models of the electromagnetic response of graphene. Our methodology not only approximates the graphene layer with a surface current, but also reformulates the governing volumetric equations in terms of surface quantities using Dirichlet–Neumann Operators. We have recently shown how these surface equations can be numerically simulated in an efficient, stable, and accurate fashion using a High–Order Perturbation of Envelopes methodology. We extend these results to the nonlocal model mentioned above, and using an implementation of this algorithm, we study absorbance spectra of TM polarized plane–waves scattered by a periodic grid of graphene ribbons.

AMS subject classifications: 78A45, 65N35, 78B22, 35J05, 41A58

Key words: Two–dimensional materials, graphene, non–local current models, electromagnetic scattering, high–order spectral methods.

1 Introduction

Over the past twenty years, the field of plasmonics has been revolutionized with the isolation and utilization of two–dimensional materials, particularly graphene. Graphene is a single layer of carbon atoms arranged in a honeycomb lattice which has striking mechanical, chemical, and electronic properties [11, 13]. It was first isolated in 2004 [26] resulting in the awarding of the 2011 Nobel Prize to Geim [12] and Novoselov [32]. At this point the literature on graphene is so vast that it is impossible to describe even a fraction

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of it here, however, we point the interested reader to the website maintained by *Nature* dedicated to the major developments in the field [24]. The authors have found the survey article of Bludov, Ferriera, Peres, and Vasilevskiy [2] and survey book of Goncalves and Peres [15] to be particularly helpful.

Among the many optical phenomena associated to graphene, the collective charge oscillations known as plasmons [17,19] are distinguished. Recently, the dispersive, nonlocal properties of these graphene plasmons have generated interest in the engineering literature [6,8,20,23,45] and the object of this contribution is to initiate this study. In particular, we describe a novel algorithm, inspired by our previous work [30], for simulating the scattering returns by a periodic array of graphene strips which takes into account the effects of nonlocality. We point out that, in addition to the optical phenomena that we have mentioned above, graphene has become indispensable in applications as diverse as energy storage [37], drug delivery and tumor therapy [39], biomedical devices [42], strain sensors [21], and membranes [25].

Before beginning our description, we point out that among the many techniques for numerically simulating structures featuring graphene (or other two–dimensional materials), simply solving the volumetric Maxwell equations in either the time domain (e.g., the Time Domain Finite Difference method [43]) or frequency domain (e.g., the Finite Element Method [18]) are natural options [9]. Typically, the graphene is modeled with an effective permittivity supported in a *thin* layer, or as a surface current with an effective conductivity at the interface between two layers [16]. In either case, commercial black–box Finite Element Method (FEM) software such as COMSOL Multiphysics™ [5] is typically utilized, however, these simulations are quite costly due to their low–order accuracy and volumetric character.

In our recent contributions [29,30] we described a method which overcomes these drawbacks by not only restating the frequency domain governing equations in terms of *interfacial* unknowns, but also describing a highly accurate, efficient, and stable High–Order Spectral (HOS) algorithm [14,40,41]. A feature of our algorithm is that, in order to close the system of equations, surface integral operators must be introduced which connect interface traces of the scattered fields (Dirichlet data) to their surface normal derivatives (Neumann data). Such Dirichlet–Neumann Operators (DNOs) have been widely used and studied in the simulation of linear wave scattering, e.g., interfacial formulations of scattering problems [27,29–31].

The object of our study is the plasmonic response that can be generated by graphene and, as in many photonic devices, structural periodicity is one path. This can be accomplished in several ways, and in one of our earlier papers [29] we focused upon graphene deposited on a periodically corrugated grating. In this the height/slope of the corrugation *shape* was viewed as a perturbation parameter and the resulting High–Order Perturbation of Shapes (HOPS) scheme sought corrections to the trivially computed flat–interface, solid graphene configuration. However, it is much more common to create a structure with *flat* interfaces upon which periodically spaced ribbons of graphene are mounted. In the paper [30] we modeled this configuration by multiplying the (con-