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Well-organized MZT-ME-PML Approach for THz BP Metasurface Implementations

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Abstract. Via adopting the matrix exponential (ME) approach, efficient and tight complex-frequency-shifted perfectly matched layer (CFS-PML) formulations using the matched Z-transform (MZT) method are well organized and proposed to truncate the monolayer black phosphorous (BP) metasurface problems in the infrared regime. Due to introducing ME approach, the proposed MZT-ME-PML develops into the compact first-order differential matrix form used to the circumvent convolution manipulations, the variable replacements, or the formulation rearrangements during the mathematical derivations. Furthermore, the MZT- ME-PML can not only flexibly truncate arbitrary materials due to using the $\boldsymbol{DB}$ constitutive relation, but efficiently attenuate evanescent waves and reduce late-time reflections with the CFS scheme. Besides, in view of the discretization effect on Terahertz (THz) BP metasurface implementation, the MZT technique is added deliberately into this proposal in that it is more suitable for simulating fine structures. Finally, the ME-based proposal can maintain high absorption when it comes closer to terminate finite-difference time-domain (FDTD) domains so that smaller physical regions can be applied, leading to palpable improvements in memory and CPU time. The three-dimensional (3D) numerical simulations on monolayer BP THz problems have been carried out to illustrate the validity and accuracy of the proposal.

AMS subject classifications: 78M20, 78A10, 15A16

Key words: Black phosphorous, complex-frequency-shifted perfectly matched layer, finite-difference time-domain, metasurface, matched Z-transform, matrix exponential.

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1 Introduction

The angstrom-scale two dimensional layered materials (2DLMs) [1, 2] have attracted a tremendous amount of interests from semiconductor device engineers, condensed matter physicists, chemists, and material scientists. As well known to all in the advanced materials community, they have great promise for applications in photonics [3–9], electronics [10–18], thermoelectrics [19,20], and sensing [21,22]. Due to wan der Waals (vdW) forces that weakly bounded to the adjacent monolayers of 2DLMs, such as graphene, black phosphorous, hexagonal boron nitride, transition metal dichalco-genides (TMDs), they are often called vdW materials. Almost all optical properties of vdW materials, like optical resonances due to oscillations of surface plasmon polaritons, and light emission/lasing and excitons generated in the semiconductors, can be found in their 3D counterparts [23].

As an emerging member of 2DLMs, Black phosphorus (BP) is among the hottest research topics of 2D material family due to its unique characteristics, such as high carrier mobility, strong light-matter interaction in the mid- and far-infrared range, and high degree of band anisotropy [24, 25]. A peculiar characteristic of the BP, namely the in-plane anisotropy, makes it different from graphene and TMDs with in-plane isotropy. It's because of a unique puckered layered atomic structure of the BP with two inequivalent geometrical directions, i.e. the armchair edge (perpendicular to the atomic ridges) and the zigzag edge (parallel to the atomic ridges).

The single layer BP metasurface research in the open-domain finite-difference time-domain (FDTD) numerical simulation is scarcely mentioned in researches on 2DLM. Specifically, investigations on the absorption performance of the perfectly matched layer (PML) for 3D 2DLM metasurface problems in the infrared regime are quite rare in the literatures.

As a highly effective tool for solving the Maxwell's equations, the FDTD method has earned great popularity. It is based on a set of simple formations that avoids complex asymptotic or Green functions [26]. Presently, the FDTD method shows its power in solving numerous types of problems [27–29], such as antennas, waveguides, filters, demultiplexers, scattering, non-linear materials, and many other applications. Nevertheless, due to the limitation of computational resources, the absorbing boundary condition (ABC) is of key importance in the FDTD method to model open-region domains [30]. As a highly effective absorbing-material ABC, the PML firstly proposed by Berenger in 1994 is one of the most popular and prominent ABCs [31]. It can truncate simulation domains comprised of various materials, including inhomogeneous, dispersive, anisotropic, and even nonlinear media.

As the consecutive evolution of Berenger's seminal work, the stretched coordinate PML (SC-PML) and Uniaxial PML (UPML) are proposed by Chew et al. [32], and by Sacks et al. [33], respectively. These two alternative PML implementations are so practical that they have led to widespread applications. However, as presented in [34, 35], these conventional SC-PML and UPML are still inefficient for reducing late-time reflections