Simulation of nanophotonic nonlinear metasurfaces

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***Abstract*—Nonlinear metasurfaces offer a new approach for nonlinear optics, with limitless design potential, very small footprints, no phase matching requirements, all with enhanced and controlled nonlinear processes. Alongside this is the need for simulation tools that can exploit this design potential and understand the properties of such devices. In this talk, we will review some of the most used methods in nonlinear nanophotonics simulations, and present some examples of such simulations of nonlinear plasmonic metasurfaces.**

***Index Terms*—metasurfaces, plasmonics, nonlinear optics, computational electromagnetics**

I. INTRODUCTION

Metasurfaces are engineered surfaces containing nanoscale elements that can exhibit exotic properties not found in nature. The nanoscale elements, or “meta-atoms” [1] are typically arranged on a lattice, and can be composed of various materials, including metal, dielectrics, and/or semiconductors. Made possible due to the development of advanced nanofabrication techniques, metasurfaces afford the possibility to control light scattering. For this reason, they have been investigated for many applications, including beam shaping [2], biosensing [3] and for creating colour [4].

Recently metasurfaces have been investigated in the nonlinear regime, as they confer many advantages over natural nonlinear materials [5]. First, the ultrathin surface geometry means that phase matching is all but guaranteed, and integration into all-optical circuits is possible. The weak nonlinear response of traditional nonlinear optical materials means that large volumes are required to accumulate enough nonlinear signal, which in turn means that challenging phase-matching schemes become a necessity. Second, metasurfaces allow for nonlinear optical properties to become enhanced. For example, the enhancement of near fields in and around meta-atoms, as reported in plasmonic [6] and dielectric [7] nanostructures, can significantly enhance nonlinear processes in such hot spots. Third, they afford the possibility for complete control of the nonlinear process, by controlling the amplitude, phase, and polarization of the linear field driving the nonlinear process via the shape, material composition, and precise arrangement of meta-atoms on the surface.

Plasmonic metasurfaces exploit localized surface plasmon resonances in metallic nanostructures, and have been applied to enhance second [8] and third [9] harmonic generation, difference frequency generation [10], four-wave mixing [11], and high harmonic generation (HHG) [12]. While dielectric/semiconductor meta-atoms typically create lower near field enhancement than plasmonic ones, they are also much less lossy and typically have larger mode volumes which may lead to higher efficiencies. Dielectric metasurfaces have been applied to enhance several nonlinear processes [13], and HHG [14]. Controlling the phase and polarization of the nonlinear signal allows one control over the far field nonlinear beam. For example, in [15], the nonlinear phase and polarization were controlled by placing nanostructures at a different rotation angle on the lattice of a proposed metasurface, creating a high order OAM beam.

Accompanying the progress in nonlinear metasurfaces, and their seemingly infinite design space, is the need for simulation tools that properly model them. This allows one to design the metasurfaces to have the exotic properties being sought, to switch materials and change geometries at will, and to optimize designs without costly and time-consuming trial and error in the lab. Simulations provide insight into the nonlinear generation process itself, difficult to glean from far fields, such as from what material the nonlinear signal originates in a complex multi-material meta-atom [16].

II. NONLINEAR SIMULATIONS

While there is a plethora of simulation work and numerical techniques for linear nanophotonics, there is decidedly less for the nonlinear regime, which does present some unique challenges. Analytical solutions can be found for simple systems but there are few such cases. Computational methods usually are required, and these have included the finite element method [17], the surface integral equation method [18], the volume integral method [19], and time-domain methods such as finite-diference-time-domain (FDTD) [16], [20]. We describe two commonly-used approaches below.

A. Two-steps approach

Here the nonlinear problem is solved by performing (at least) two linear simulations in the frequency domain, one for the incident linear field (or fields), and one for the nonlinear field. This approach is only valid when the nonlinear signal is weak enough that it does not effectively perturb the incident linear field, that is, the undepleted pump approximation applies.

In one method, the field distribution of the incident field at the desired pump frequency is calculated. In the next step,

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the nonlinear polarization is calculated using the incident field from the first simulation. This nonlinear polarization is then used as the source in Maxwell's equation at the relevant nonlinear frequency.

Another method, recently applied to nonlinear metamaterials [21], stems from the Lorentz reciprocity theorem. It consists of two linear simulations: one to calculate the field distribution at the pump frequency, and another to calculate the field distribution at the nonlinear frequency. The nonlinear signal is determined by the overlap of the nonlinear polarization (determined from the pump field distribution) and the nonlinear field distribution.

B. Direct nonlinear generation approach

In circumstances where the depleted pump approximation doesn't apply, the time dynamics are of interest, and/or there is broad spectrum excitation, the two-steps approaches are not appropriate. We consider here FDTD, as it is the most widely used method in nanophotonics, because it is relatively straightforward to implement and it is very versatile in that it can be made to simulate almost any material and any geometry. Importantly here, nonlinear optical processes can be directly implemented within the code. One of its drawbacks is that there can be large computational requirements, but given that it is also very suitable for parallel processing due to its almost linear scalability [22], this can be mitigated with appropriate computational resources.

One method is to incorporate nonlinear polarizations within an existing auxiliary differential equation method (ADE) implementation [20], [23]. The ADE method is used to simulate linear dispersion, via Drude, Lorentz, and Drude+2 critical points models [22], [24], to name a few, and introduces an additional updating equation for the polarization field in the leapfrog FDTD algorithm. In the case of nonlinearity, the nonlinear polarization term can have arbitrary complexity, it can be dispersionless, dispersive, and can even incorporate the hydrodynamic model which describes the current density of the electrons in the medium and includes nonlinear terms as well [23], [25], [26].

In this talk, we will give more details on the approaches described here, and present a few examples from our research that illustrate both approaches for plasmonic metasurfaces.

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