Freeform inverse design in photonics by re-thinking the questions

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Abstract— **Recent developments in computational freeform inverse design have provided a fertile landscape of structures and topologies for nanophotonics. However, simply dumping millions of parameters into a simulation can easily lead to intractable computational problems. Fortunately, a given engineering problem often admits many different mathematical formulations, and by carefully matching the formulation to the available electromagnetic solvers and optimization algorithms one can set the stage for extraordinarily flexible automated design. In this talk, we will show that, with careful consideration and reformulation of the design problem, powerful inverse design techniques can be successfully applied to a multitude of interesting problems with rich physical behavior, ranging from light confinement in nonlinear multi-resonant cavities, robust bandgap maximization in 3D photonic crystals to beam-forming and manipulation through multi-layered metasurfaces.**

The advent of nano-structured photonic devices with functionalities beyond conventional bulky optics has engendered robust interest and rapid progress in the topic of photonic optimization. Recently, freeform inverse design strategies, based on topology optimization, have gained increasing attention due to their ability to discover complex geometries and unprecedented functionalities that may be difficult to realize through conventional intuition alone [1], [2]. Such techniques typically consider every pixel or voxel in a design region as a degree of freedom and are capable of efficiently exploring a very large design space by exploiting the analytical derivative information of the specified objective and constraint functions. However, for many important problems in optics and photonics, the most obvious formulations might not be the most suitable ones for optimization nor might they be immediately amenable to fast electromagnetic solvers, which are a crucial component of every large-scale inverse design method. In such cases, a careful analysis of the underlying physics and the mathematical nature of the problem often reveals novel alternative formulations that can be more efficiently handled by available numerical techniques. In this talk, we will discuss a variety of carefully formulated inverse design problems, ranging from light confinement in nonlinear multi-resonant cavities, robust bandgap maximization in 3D photonic crystals to beam-forming and manipulation through multi-layered metasurfaces

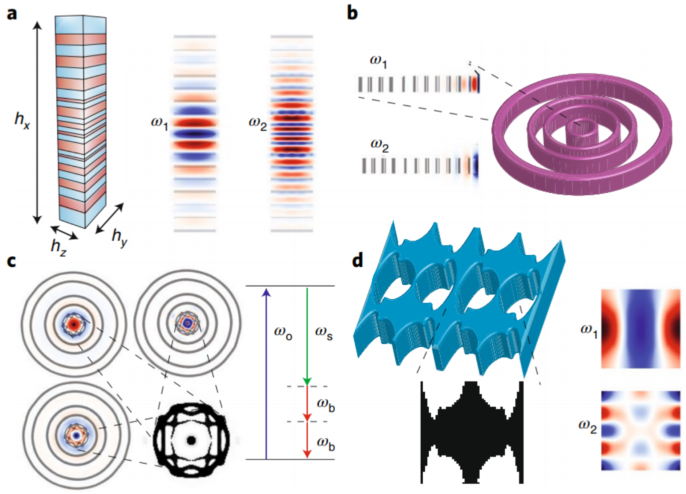

Fig. 1. Topology optimized multi-resonant photonic structures for nonlinear frequency conversion. (a,b) A micropost cavity (a) and a multi-track ring resonator (b) for enhanced second harmonic generation [3], [4]. (c) A 2D cavity exhibiting a non-trivial topology for enhanced third-order difference frequency generation [4]. (d) unit cell of a topology-optimized photonic crystal slab for enhanced second harmonic generation [5].

Confining light in a small volume over a long period of time is a central requirement for many important nanophotonic applications. As such, optical microcavity design poses a significant challenge that welcomes large-scale optimization strategies. However, the associated eigenproblem does not lend itself well to brute-force optimization due to numerical issues associated with differentiation and tracking of eigenmodes [6]. Instead, cavity optimization can be judiciously recast into a maximal scattering problem by realizing that a cavity mode is succinctly characterized by the local density of states (LDOS) which is, in turn, proportional to the power radiated by a point dipole source positioned at the desired modal center. Meanwhile, the computational cost and convergence characteristics of problems involving scattering through resonant systems can be dramatically improved using window functions and complex-frequency deformations when the objective function is analytic. First, the objective is multiplied by a meromorphic function peaked around the frequency bands of interest (for example, a Lorentzian). By analytically continuing to the complex plane, the entire objective is then obtained from the spectral residues of the window function, requiring far fewer calculations [6]. These notions can be further extended to the concept of nonlinear LDOS and fruitfully applied to the even more challenging problem of nonlinear frequency conversion involving multi-resonant cavities (Fig. 1) which require not only light confinement at mutliple widely separated frequencies but also maximal spatial overlap between modes for efficient frequency conversion [3], [4], [5].

While LDOS formulation may be more suitable for cavity

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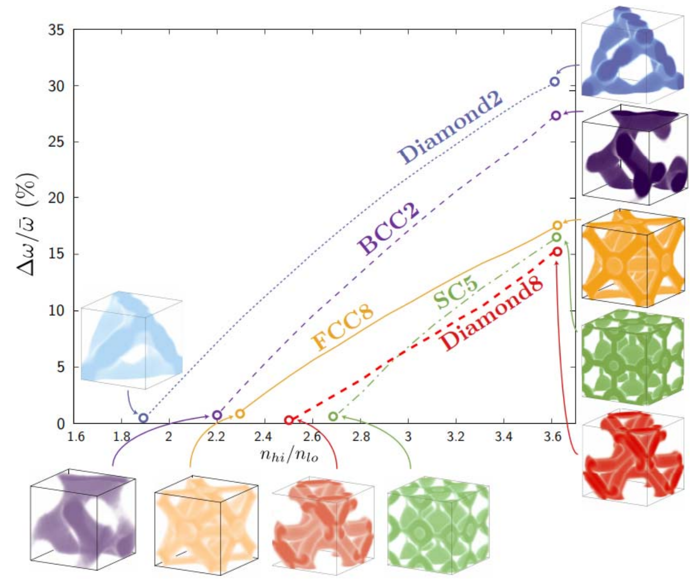

Fig. 2. Robust topology optimization of photonic crystal bandgap. Optimal crystal structures for various symmetry groups are revealed against arbitrary index contrast [7].

optimization, there may be situations where one cannot avoid dealing with eigenmodes. One such problem is photonic bandgap maximization (Fig. 2). The key to handling such a problem is to determine and isolate the dominant eigenmodes and, subsequently, limit the total optimization problem to more tractable finite-dimensional subspaces. Employing these subspaces as a basis set for describing arbitrary modal evolutions, and reparametrizing the problem with the help of a few extra decision variables, one arrives at a novel semidefinite program for photonic bandgap optimization [7].

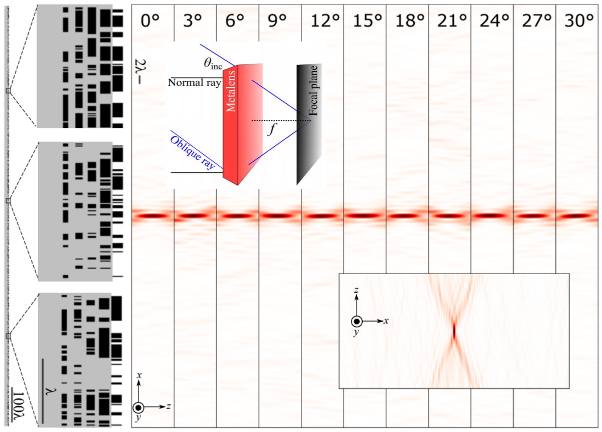

Fig. 3. Topology-optimized multi-layered 2D metalens concentrator which can combine 11 incident angles to a single focus [8].

While nanophotonics is known to enable on-chip *intra-device* near-field manipulation of light, it has also proven a versatile platform for far-field beam shaping and propagation, particularly in the context of metasurfaces [9]. Although inverse design methods have been recently proposed for metasurfaces, these methods so far either rely on pre-compiled libraries of fixed-form primitive geometric elements [10] or are limited to smaller areas [11]. Meanwhile, large-area metasurfaces are typically modeled by a locally periodic approximation (LPA) in which the metasurface is divided into computationally tractable independent unit cells with periodic boundary conditions [9]. Combined with LPA, we have extended freeform inverse design techniques to large-area metasurfaces, single or multi-layered, over 10^5–10^6 degrees of freedom in two and three dimensions, 100–1000+ wavelengths (λ) in diameter, with 100+ parameters per λ^2 [8]. In this way, we have computationally discovered completely unexpected metasurface designs for challenging multi-frequency, multi-angle problems, for example, the design of a multi-layered metalens that can concentrate incoming light at multiple incident angles to the same focus (Fig. 3).

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