Nonlinear generalized source method for modeling bulk and surface second harmonic generation in diffraction gratings

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We present a new numerical method for the analysis of second-harmonic generation (SHG) in two-dimensional (2D) diffraction gratings containing either centrosymmetric or non-centrosymmetric quadratically nonlinear materials. Our method incorporates the bulk (local) nonlinearity characterizing non-centrosymmetric materials and both surface (local) and bulk (non-local) nonlinearities that correspond to centrosymmetric media. Our approach is based on the generalized source method (GSM), which is an efficient numerical method for solving the (linear) problem of diffraction by periodic structures of arbitrary shape. The GSM can be described as a three-step algorithm: For a given excitation at the fundamental frequency the linear field response is computed using the linear GSM. This field gives rise to a nonlinear source polarization at the second harmonic (SH) frequency. A nonlinear extension of the GSM incorporates the nonlinear polarization as an additional source term and is used to compute the nonlinear near- and far-field response at the SH.

The dependence of the SH source polarization on the fundamental field is related to the symmetry properties of the nonlinear material: non-centrosymmetric materials lack inversion symmetry and therefore allow local even-order SHG in the bulk of the material, whereas this process is ruled out in centrosymmetric materials. The inversion symmetry of centrosymmetric materials is broken at their surface whence they allow local surface SHG. Additionally, centrosymmetric materials contribute to the nonlinear source polarization by means of a nonlocal (bulk) excitation. The presented numerical method seamlessly incorporates all these quadratic nonlinear processes in a single formalism and is therefore applicable to a wide variety of periodic devices composed of nonlinear materials. To illustrate this flexibility, we apply the nonlinear GSM to 1D and 2D periodic metallo-dielectric resonant structures exhibiting bulk and surface SHG and investigate the relative contribution of the bulk and surface nonlinearity to the nonlinear optical response at the SH.
Evolutionary design of linear chains of metallic nanoparticles for field enhancement and localization effects

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Periodic and disordered metallic nanoparticle arrays that support surface plasmons (SPs) have been extensively researched. SP excitations, which can be confined to sub-diffraction limited volumes, can play important roles in the manipulation of light through metallic nano-arrays. Here we employ a self-consistent coupled dipole model\(^1\) to study field enhancement and light localization effects in linear chains of nanoparticles that can either be periodic or disordered. We investigate the optimisation of enhanced field effects and plasmon propagation lengths with different polarisations and nanoparticle separations using an evolutionary algorithm\(^2\) (EA). EAs are commonly applied to design optimisation tasks and are used to generate novel designs that solve a problem by generating solutions based on the principles of natural selection; the characteristics of a solution that optimises the problem well will be propagated to future solutions in favour of the characteristics of less successful solutions, until eventually a good approximation to the best possible solution parametrisation is identified.

We will discuss how an EA can be used to optimise the placement of symmetric nanospheres and how, building on this initial approach, the inherent flexibility of an EA can be exploited to add degrees of freedom to the optimisation problem. For example, rather than just optimising the location of the nanospheres in the chain alone, later experiments will explore the efficacy of elliptically-shaped nanoparticles; to do this, the EA seeks the optimal aspect ratio of the nanoparticles, as well as optimising their position along the SP-coupled chain array. The ultimate goal of this work is to produce a framework that can be applied to the generation of bespoke nanoparticle arrays to produce enhanced field effects that are suited to particular tasks.

Thursday 4 September
Session 1: Computational Photonics (09:30 – 09:45, Huxley LT 341/342)

Optical snowflakes: from Fresnel diffraction to a new class of unstable resonator
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Unstable cavity lasers are linear systems with inherent magnification. It has long been known that the eigenmodes of unstable strip resonators have fractal characteristics [Karman and Woerdman, Opt. Lett. 23, 1901 (1998)], possessing proportional levels of detail across decimal orders of spatial scale. Kaleidoscope lasers are generalizations of the strip resonator to fully two-dimensional (2D) transverse geometries where the feedback mirror has the shape of a regular polygon [McDonald et al., JOSA B 17, 524 (2000)]. Here, we propose a new class of unstable resonator: the snowflake laser. This novel system has a feedback mirror whose shape matches a classic fractal curve – the von Koch snowflake (an iterated function system involving self-similar sequences of equilateral triangles). As such, we have now designed a cavity whose eigenmodes are inherently fractal, and where successive round trips involve the interplay of that fractal light beam with a fractal aperturing element.

In this presentation, we show how the 2D virtual source (2D-VS) method deployed for kaleidoscope geometries [Huang, Christian, and McDonald, JOSA A 23, 2768 (2006)] can be applied to modelling the snowflake laser. A key development has been an exact analytical reformulation of the Fresnel diffraction problem for snowflake apertures using a line integral [Hannay, J. Mod. Opt. 47, 121 (2000)]. In contrast to the traditional Fox-Li approach (based upon paraxial ABCD matrix modelling and fast Fourier transforms), the 2D-VS approach permits entire families of eigenmodes to be obtained from a single calculation (from lowest loss through the hierarchy of higher-order modes). Furthermore, arbitrary cavity parameters (equivalent Fresnel number and round-trip magnification) may be specified and patterns calculated to any prescribed accuracy. A selection of mode patterns and eigenvalue spectra will be reported for increasing iterations of the von Koch snowflake (as the aperture tends towards a fully-developed fractal), and computational challenges highlighted.
Diffraction of fractal light by simple apertures

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Berry's seminal work from over three decades ago [J. Phys. A 12, 781 (1979)] established that plane waves scattering from complex objects (e.g., a transparent mask with a random fractal phase modulation) may acquire fractal characteristics in their statistics. Here, we consider the diametrically-opposing paradigm for optical complexity: the diffraction of a fractal wave from a simple object. Surprisingly, this rich and potentially highly fertile research ground has received almost no attention in the literature to date.

In this presentation, we will report on very recent research results concerning the scattering of fractal light from simple apertures. Attention is paid to two historic configurations that underpin both theoretical and experimental studies of diffraction: (i) a single infinite edge, and (ii) a single infinite slit (constructed from a pair of parallel edges). While classic analyses considered normally-incident plane-wave illumination, the novelty of our approach lies in accommodating an incident optical field that possesses a very broad spatial bandwidth (i.e., a waveform whose Fourier spectrum extends over decimal orders of pattern scalelength). Exact mathematical descriptions of near-field (Fresnel) diffraction patterns have been obtained using a prescription based on Young's edge waves [Silverman and Strange, Am. J. Phys. 64, 773 (1996)]. Furthermore, far-field (Fraunhofer) predictions emerge asymptotically in the limit of vanishing Fresnel number. These preliminary analyses have been supplemented by further considerations, namely the propagation of fractal wavefronts that have been modulated by finite-waist beams. Key – and somewhat unexpected – results will be presented that address, for the first time, the effect of finite aperturing on the propagation of scalar fractal light waves. Our findings have implications for, and applications in, a diverse range of fields such as fractal antenna engineering [Werner and Ganguly, IEEE Antenna Prop. Mag. 45, 38 (2003)] and surface-roughness measurement techniques [Wada et al., Opt. Commun. 166, 163 (1999)].
Thursday 4 September
Session 1: Computational Photonics (10:00 – 10:15, Huxley LT 341/342)

Light confinement in hyperuniform photonic slabs: High Q cavities and low-loss waveguides
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Hyperuniform disordered photonic structures are a new class of photonic solids, which display large, isotropic photonic band gaps (PBG) comparable in size to the ones found in photonic crystals. The existence of large band gaps in HUDs contradicts the long-standing intuition that Bragg scattering and long-range translational order is required in PBG formation, and demonstrates that interactions between “Mie-like” local resonances and multiple scattering can induce PBGs on their own. The hyperuniform disordered structures combine advantages of both statistical isotropy due to disorder character and controlled scattering properties due to hyperuniformity (due to constraints imposed on the disorder) and uniform local topology.

The structures are designed by employing a centroidal tessellation of a hyperuniform point pattern to generate a “relaxed” trihedrally coordinated network lattice, whose vertices are connected with Si dielectric walls of variable thickness. In the resulting network architecture point-like and planar defects are introduced by filling up network cells.

Using finite-difference time domain and band structure simulations, we demonstrate efficient confinement of TE polarized radiation and high-Q optical cavities and low-loss waveguides in the resulting planar HUD architectures. For two-dimensional structures, quality factors exceeding \( Q > 10^9 \) are achieved. We further show that for 3D finite-height photonic slabs high quality factors exceeding \( Q > 20,000 \) can be maintained. Moreover, a multitude of cavity modes can be obtained, which can be classified according to the symmetry (monopole, dipole, quadrupole, etc.) of the confined electromagnetic wave pattern.

Our results put to rest the presumption that disorder would induce significant out of plane scattering in disordered structures as compared to their periodic counterparts and demonstrate the ability of disordered HUD PBG materials to serve as a general-purpose design platform for integrated optical micro-circuitry.