Inverse-Designed Metasurfaces for High-Efficiency Sum Frequency Generation

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Sum-frequency generation (SFG) is a fundamentally important second-order nonlinear process with many applications spanning from changing the wavelength of optical sources to spectroscopy. Recent advances in nanotechnologies facilitated the development of ultra-thin metasurfaces where optical resonators can enhance and tailor nonlinear interactions with functionalities beyond the capabilities of traditional bulky crystals [1, 2]. The metasurface designs were often obtained semi-analytically in the limiting cases of localised Mie-type modes for individual nanoresonators or nonlocal lattice resonances. We demonstrate that the largely unexplored intermediate regime may offer more flexibility in enhancing the SFG process.

We develop an inverse-design method for optimisation of high-efficiency SFG by nontrivially generalising the inverse-design approach previously applied to the case of second-harmonic generation [3]. The algorithm is based on freeform topology of the metasurface, where the gradient of the figure of merit is efficiently calculated through a series of adjoint simulations. We show a representative example of SFG optimisation for incoming photons with wavelengths of 860 nm and 1550 nm (Fig. 1a). The nonlinear material is gallium arsenide (GaAs) which is 300 nm thick. We show in Fig. 1b a 2-by-2 unit cell of our final optimised metasurface. Because the algorithm is agnostic to the underlying physics for high efficiency, e.g. quality factor and mode overlap, the structures that emerge from the optimisation are highly nontrivial. Our optimised metasurface has an SFG generation efficiency of $1 \times 10^{-3}\,\mathrm{cm^2\,GW^{-1}}$ (Fig. 1c), representing five orders of magnitude enhancement over an unpatterned GaAs film of the same thickness. We observe that the algorithm has converged to structures that peaks in SFG efficiency around the input wavelengths 1550 nm and 860 nm (Figs. 1d,e) as required. We anticipate that the inverse-designed metasurfaces may find future applications for SFG-based imaging across the infrared spectrum.

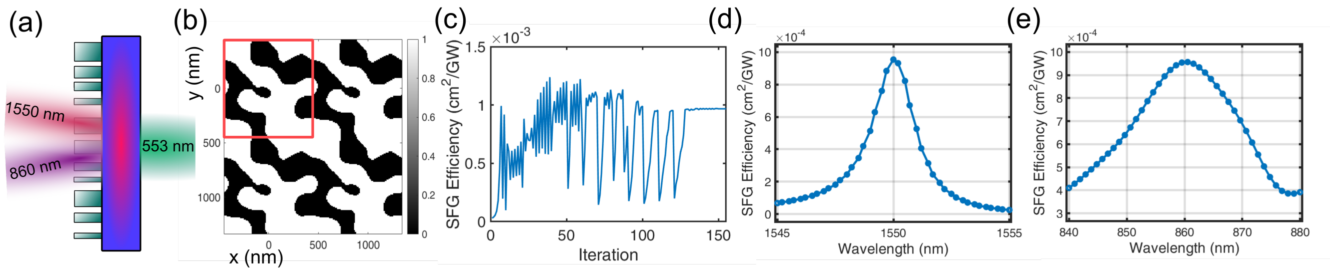

Figure 1: (a) Scheme of SFG inputs and output. (b) Final optimised structure; GaAs is shown white and air shown black. Red box outlines one unit cell. (c) Iterative increase of conversion efficiency over the topology optimisation steps. (d,e) SFG efficiency around input wavelengths 1550 nm and 860 nm respectively, while fixing the other input wavelength.

[1] C. D. Angelis, G. Leo, and D. N. Neshev, eds., *Nonlinear Meta-Optics* (CRC Press, London, 2020).

[2] T. Pertsch and Y. Kivshar, MRS Bull. **45**, 210 (2020).

[3] C. Sitawarin, W. L. Jin, Z. Lin, and A. W. Rodriguez, Phot. Res. **6**, B82 (2018).