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Plane-wave Expansion based Modelling of Linear and Non-Linear Response of Resonant Metasurfaces under Realistic Excitation Conditions

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It is generally easy to model resonance characteristics of infinitely periodic resonant metasurfaces under plane-wave excitation. However, extending this to finite size arrays and more realistic Gaussian-like excitation beams becomes complex and time-consuming. Extending the linear optical resonances to model the nonlinear optical performance also becomes cumbersome. The use of non-standard, off-axis excitation, for example using reflective objective with central obscuration are also difficult to model with existing simulation tools. Here, we report a unified approach to modelling linear and nonlinear optical characteristics of resonant metasurfaces using a plane wave expansion (PWE) method to realize gaussian excitation with any arbitrary excitation angular profile. As an example, we compare the PWE model with experimental results of linear and third-order sum-frequency generation (TSFG) from 1D gratings with double step profile supporting q-BIC resonances, which we have previously reported experimentally [1].

The PWE technique developed here in COMSOL Multiphysics uses parameters of the excitation optics (numerical aperture, the equivalent acceptance angle, θ_{NA} and any obscuration angle, θ_{obc}) as the starting point. Plane waves at different angles of incidence, θ_{inc} varying from $0 < \theta_{inc} < \theta_{NA}$ for réfractive objective and $\theta_{obc} < \theta_{inc} < \theta_{NA}$ for reflective objective incident on a single unit-cell of the metasurface with periodic boundary conditions are considered. The vectorial electric/ magnetic field components (E_i $(x, y, z, \theta, \omega)$ and, H_i $(x, y, z, \theta, \omega)$ with $i = x,y,z$) are acquired throughout the simulation region. The fields are scaled appropriately to correct the angular response with a weighing factor, $W = exp(-\theta^2_{inc}/2\theta^2_{max})$ for incident Gaussian beam. Subsequently, the total vectorial fields for the overall Gaussian excitation are calculated by taking a coherent summation of the above weighted fields at each input wavelength. The linear transmission spectra are obtained by calculating the total power (integrated Poynting vector at the monitor plane) and normalizing this with corresponding calculation in the absence of the metasurface. Non-linear optical response, such as the TSFG power spectrum is obtained by calculating the nonlinear polarization within the medium of interest and using this as the driving term to compute the field components and the corresponding integrated Poynting vector for the nonlinear signal wavelengths.

A comparison of the computed linear transmission spectrum using PWE model (blue-curve), normal incidence plane-wave (red-curve), and experimental measurement (green-curve) for narrow angular excitation (up to 3°) are shown in Fig. 1(a). A schematic of the cross-section of the metasurface unit-cell is shown as an inset. Prominent resonance dips at ~3.15 and 3.32 μm are observed with good agreement between the PWE, normal incidence plane-wave and experiments for the narrow angular spread considered. To further study the effect of central obscuration of reflective objective on transmission spectrum, PWE model (red-curve) with obscuration ($15° < \theta_{inc} < 40°$) is compared with PWE model (blue-curve) and gaussian beam exciting finite metasurface (grey-curve) without obscuration ($0° < \theta_{inc} < 40°$) are shown in Fig.1(b). A single prominent, blue-shifted resonance dip is observed at ~2.9 μm (red-curve in Fig. 1(b)). The resonance modification in the presence of central obscuration in the excitation is furthered validated by comparing the nonlinear PWE-model and experimentally measured TSFG response (both on and off the metasurface), as shown in Fig.1(c). The TSFG spectra shows a clear peak at ~2.9 μm with an enhancement of 32-times. In summary, good agreement is obtained between the PWE-model and experiments for studying the linear and nonlinear performance of the resonant metasurface.

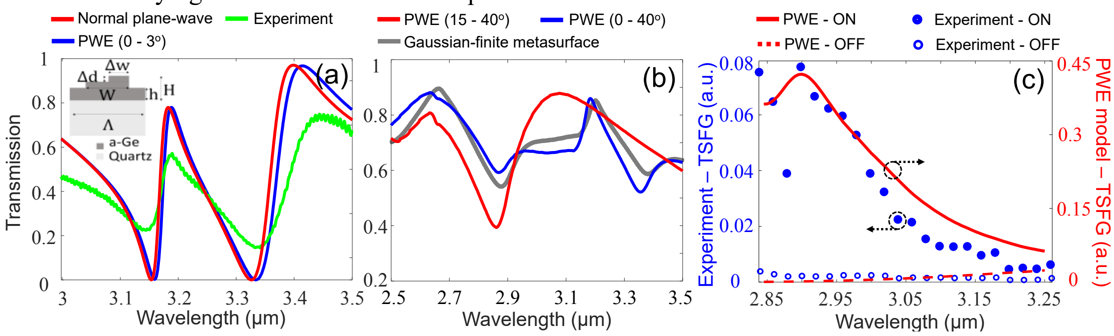

Fig. 1: (a) Experimental and simulated transmission spectra under normal incidence plane-wave and PWE model (inset shows metasurface unit-cell). (b) Transmission spectra calculated with PWE for 15-40°, 0-40° and gaussian excitation of finite metasurface. (c) Experimental and simulated TSFG spectrum shown on- and off- the metasurface.

References

[1] Lal Krishna A.S., Jyothsna K. M., Asish Prosad, Rabindra Biswas, Sruti Menon, Varun Raghunathan, "Quasi-BIC resonances in amorphous germanium zero contrast gratings with dual asymmetric step profile for mid infrared frequency up-conversion," Proc. SPIE 12011, High Contrast Metastructures XI, 1201104 (5 March 2022).