Design for Highly Efficient Nanometagratings and Theory of Extreme Subdiffraction Photon Control

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Conventional planar metasurfaces are always much larger than the wavelength level. Previous studies on extreme wavefront control based on superoscillation suggest a fundamental tradeoff between the size and efficiency of diffraction-based metasurfaces. Herein, the theory of extreme subdiffraction photon control is proposed and the abnormal wave propagation phenomenon supporting logical design for highly efficient metasurfaces of subwavelength size is pointed out. A new class of novel metasurfaces named nanometagratings is demonstrated, which is smaller than one wavelength, and manages to achieve arbitrary wavefront engineering with high conversion efficiency, enabling extreme photon control within subwavelength scale. The theoretical approach is expected to open the avenue for ultrasmall highly efficient functional metasurfaces and promises novel applications such as highly integrated on-chip quantum optical information computation.

1. Introduction

Metasurfaces are thin structured arrays that exploit advanced light–matter interactions to achieve exquisite wavefront control.[1–4] They have attracted significant attention for the ability to realize ultrathin optics with multiple conventional or nonconventional functions. However, despite different light–matter interactions they employ, most of these geometries are still based on the conventional Fourier-based planewave propagation theories[1–5] which are insufficient for describing the underlying physics of local subwavelength propagation. As well illustrated in other studies,[6,7] when the overall size of the metasurface is smaller than the wavelength, the only reasonable conclusion derived from these theories is that most of the spectrum of the finer structures falls into the evanescent region, and nearly no metastructure functioning as rather than a pinhole beyond the extreme immediate proximity can be designed.

As a result, these approaches suffer from fundamental limit on the overall scale, which must be at least several times larger than the wavelength level.[6,7] Other approaches using numerical results based on the strict electromagnetic theory encounter the similar dilemma.[3,4] that they cannot provide general physical understanding for the rational design of subwavelength-sized metasurfaces.

The concept of superoscillation refers to the abnormal fluctuation phenomenon that the local spatial frequencies exceed the highest wavenumber of the entire field.[8–10] It was originally defined in terms of the quantum weak measurements by Aharonov[11] and was later developed and extended to optics by Berry.[12] Researchers have observed the superoscillatory nature of a complete set of band-limited functions called prolate spheroidal wave functions (PSWFs),[13–15] which suggests that a subwavelength-sized planar metastructure can be formed, with which the spectrum of its finer structures still lies in the propagation band. However, conventional wisdom based on the Fourier-based planewave propagation theories has also suggested that the efficiency of such metasurfaces is extremely poor, as strong sidelobes capturing almost all the energy passing through the boundary are always in company with these superoscillatory features.[16] Moreover, this “energy leakage” is known to be fundamentally related to the “space-bandwidth product” of these superoscillatory functions, suggesting that it will become much more severe when the size of the metasurfaces is small, and there is a fundamental tradeoff between the size and the overall conversion efficiency of any diffraction-based metasurfaces.[14]

Here, we propose the theory of extreme subdiffraction photon control. Contrary to the above conventional believes, we point out the abnormal propagation phenomenon that arbitrary subdiffraction features without any sidelobe can be generated beyond the near field by careful tailed subwavelength-sized boundaries, which enable rational design for general highly efficient ultrasmall metasurfaces. We proposed the concept of a new class of metasurfaces named “nano metagratings”[11,17] which are planar metasurfaces smaller than one wavelength, and manage to realized arbitrary wavefront engineering with near-unitary efficiency within subwavelength scale. We demonstrate that the structures can be formed by arrays of fine elements not exceeding the current fabrication limitations. Given the previous works on quantum information processing with conventional large-scale optics,[18–23] we show that these metasurfaces can be used...
to achieve optical quantum information processing in subwavelength scale. The theory and the designing approach are expected to open the avenue for highly efficient nanosize metasurfaces, which promise novel applications such as highly integrated on-chip optical classical or quantum computation.

2. Theory and Results

The typical situation that we address here is presented in Figure 1: a monochromatic coherent field with a wavelength \( \lambda = 2\pi/k_0 \) irradiates a 1D nanoscale metasurface and generates a transmitted field \( E(x,z) \), which satisfies the vector Rayleigh–Sommerfeld integral\(^{[26]}\)

\[
E(x_i, z) = \frac{-1}{2\pi} \int \frac{E_x(x_0, 0) \left[ \frac{\partial G(r)}{\partial z} \hat{x} - \frac{\partial G(r)}{\partial x_i} \hat{z} \right]}{r} \, dx_0
\]  

(1)

where \( G(r) = \exp(ik_0r)/r \) is the Green’s function, \( x_i \) and \( x_0 \) are the spatial coordinates on the image and the object planes, respectively, and \( \hat{x}, \hat{z} \) are the unit vectors (as shown by Figure 1). Here we only consider the vector-transmitted electric field in a 2D plane, reflection, and the more complicated 3D case can be worked along the same line.\(^{[1]}\) Despite the specific light–matter interaction of the fine elements, we focus closely on finding such a boundary function \( E_x(x_0, 0) \), that is zero outside a given small region on the object plane

\[
E_x(x_0, 0) = 0, |x_0| > D/2
\]  

(2)

where \( D < \lambda \) and can produce arbitrary complex diffraction patterns in the subwavelength diffraction region beyond the near field.

We stop for a few seconds to take a close look at the problem encountered by the conventional theories. We start with a simple case. Figure 2a-c shows the propagation results of a typical periodic subwavelength grating structure. As well understood by the Fourier-based planewave propagation theories, as the overall size of the structure is less than the wavelength, most of the spectrum of the finer structures falls outside the propagation band, and the characteristic diffraction pattern formed by the evanescent components disappears quickly beyond the near field. The near-field condition is generally recognized to be \( z < \lambda(D/2\lambda)^2 \) (or \( r < \lambda(D/2\lambda)^2 \)),\(^{[5-7,26,27]}\) which is quadratically proportional to \( D/2\lambda \). Therefore, conventional theories have suggested that no practical metastructure functioning as not a pinhole can be designed when \( (D/2\lambda) < 1 \).

Theories on extreme wavefront control based on the superoscillatory nature of the light field have provided deeper understanding to the problem. The PSWFs \( \psi_n(c, x) \) are a complete set of band-limited functions that are orthogonal in the interval \( [-D/2, D/2] \) and across the whole range \( (-\infty, \infty) \). They are initially developed by Slepian and Pollak to treat problems of information compression\(^{[28–31]}\) and recently recognized by Huang and Zheludev as superoscillatory functions that support far-field super-resolution without evanescent waves.\(^{[13]}\) They share the important property that the finite Fourier transform of each of them is the scaled version of itself in the whole range \( \omega \in (-\infty, \infty) \)\(^{[8,14]}\)

\[
\int_{-D/2}^{D/2} dx \, \psi_n(c, x) e^{i\omega x} = i^n \sqrt{\frac{\pi \lambda_n D}{\Omega}} \psi_n (c, \omega D/2\Omega)
\]  

(3)

where \( c = \Omega D/2 \) is the space–bandwidth product, and \( \lambda_n \) is an energy ratio, defined as

\[
\lambda_n = \frac{\int_{-D/2}^{D/2} dx |\psi_n(c, x)|^2 dx}{\int_{-\infty}^{\infty} dx |\psi_n(c, x)|^2 dx}
\]  

(4)

Equation (3) indicates that the spectrum of these functions in the interval \( [-\Omega, \Omega] \) is identical to themselves, and subwavelength details can be thus preserved at the far field when \( \Omega < k_0 \). However, it is also well known by the optical society that these superoscillatory functions introduce strong sidelobes outside the prescribed field of view, especially when the space–bandwidth product \( c = \Omega D/2 \) is small. When \( n > 2c/\pi \) (another important parameter called the Shannon number),\(^{[15]}\) \( \lambda_n \) soon tends to 0 (known as the step-like behavior of \( \lambda_n \)), meaning that a large portion of the energy will fall outside the prescribed field of view, and there is a fundamental tradeoff between the size and the efficiency of these metasurfaces.\(^{[14]}\)

![Figure 1](https://www.advancedsciencenews.com)  

Figure 1. Schematic diagram of the addressed scenario of subwavelength propagation.
While these conclusions have been reasoned from the conventional Fourier-based planewaves propagation theories, here, we argue that under the framework of proper subwavelength propagation theory, it is possible to find an exact space–bandwidth product $\beta$, that all the sidelobes are pushed to the evanescent region, so that all energy is preserved in the whole field of view. Expand $r(x_n)$ in Equation (1)

$$r(x_n) \approx r_0 - x_n \sin(\theta_0) + o(x_n^2)$$

In the study by Gao et al.,\cite{7} it has been illustrated that for propagation beyond the immediate proximity of the structures with low 0-order momentum, it is sufficient to preserve the 0-order and the first-order approximation of Equation (5) in the amplitude term and the phase term, respectively, in Green's function in Equation (1), which yields\cite{7}

$$E \approx A(r_0, \theta_0) F(\omega)$$

**Figure 2.** Profiles of the grating functions and their propagation results, $D = 0.5\lambda$, $X = 2x_0/D, X' = \sin(\theta_0)$. a–c) Propagation results of a typical periodic grating and its profile. (a) $|E_x|$ in arbitrary unit. (b) $|E_z|$ in arbitrary unit. (c) The grating function $E_x(X)|_{0 \to 0}$ (the black solid line). It’s absolute value (the black dashed line), the propagation results at $r_0 = 2.5\lambda$ ($|E_x(X')|_{0 \to -2.5\lambda}$: the yellow solid line; $|E_x(X')|_{0 \to -2.5\lambda}$: the red solid line). d–f) Propagation results of a space-limited PSWF $\psi_n(c, x)$, $c = 0.5\pi, n = 4$. d) $|E_x|$ in arbitrary unit. e) $|E_z|$ in arbitrary unit. f) The profile of $\psi_n(c, X)$ (the black solid line), its absolute value (the black dashed line), and the propagation results at $r_0 = 2.5\lambda$ ($|E_x(X')|_{0 \to -2.5\lambda}$: the yellow solid line; $|E_z(X')|_{0 \to -2.5\lambda}$: the red solid line).
where
\[ A(r_0, \theta_0) = \frac{-1}{2\pi} \left( \frac{ik_0}{r_0} - \frac{1}{r_0^2} \right) \left[ x \cos(\theta_0) - z \sin(\theta_0) \right] e^{ikr_0} \] (7)
is an amplitude term independent of \( x_0 \), and
\[ F(\omega) = \int_{-\infty}^{\infty} E_x(x_0) e^{-i\omega x_0} dx_0, \omega = k_0 \sin(\theta_0) \] (8)
is the Fourier transform of the boundary function \( E_x(x_0, 0) \) itself (please also refer to the Supporting Information Document II for further discussions on approximation). Equation (6), together with Equation (3), thus suggests the abnormal propagation phenomena that cannot be reasoned by conventional Fourier-based planewave propagation theories (even though they are strict and correct): when \( (D/\lambda) < 1 \) and \( c = Dk_0/2 \), the far-field distribution of each \( \psi_n(c, x) \) is identical to itself in the whole field of view \( \theta_0 \in (-\pi/2, \pi/2) \), and all sidelobes outside the interval \([-\Omega, \Omega]\) are pushed to the evanescent region so that all energy is preserved. Figure 2d-f shows a vivid example for clear illustration. As clearly shown, both the electric components show propagation invariance for the whole field of view \( \theta_0 \in (-\pi/2, \pi/2) \). No undesired side-lobe appears, and the propagation results fit the approximation (Equation (6)) well when \( r_0 = 5D = 2.5\lambda \) (Figure 2f). The differences between the two electric components and the boundary are introduced by the vector term \( [x \cos(\theta_0) - z \sin(\theta_0)] \), as indicated by Equation (6). In addition, as no energy is leaked outside the propagation band, the number of the usable \( \psi_n(c, x) \) should no longer be limited to the well-known Shannon number \( [14,15] \) which is also related to the step-like behavior of the energy ratio \( \lambda_n \).

We note again that PSWFs are a complete set of orthogonal functions. Therefore, it is in principle that we can reconstruct any desired wavefront beyond the immediate proximity with unitary energy conversion efficient, without a limited field of view. Our numerical results further suggest that propagation results of a finite number of \( \psi_n(c, x) \) still show good orthogonality even within subwavelength radius. Figure 3 shows the correlation matrix of the propagation results of the first 13 orders of PSWFs at \( r_0 = 1\lambda, 0.75\lambda \), respectively. Each element of the matrix is calculated by

\[ \Gamma_{mn} = \int_{-1}^{1} \text{Re}\{E_m^*(r_0, \theta_0) \cdot E_n(r_0, \theta_0)\} d\sin(\theta_0) \] (9)

where \( E_i(r_0, \theta_0) \) is the vector propagation result of \( \psi_{q-1}(c, x) \), \( q = 1, 2, \ldots, 13 \), normalized to

\[ \int_{-1}^{1} \|E_i(r_0, \theta_0)\|^2 d\sin(\theta_0) = 1 \] (10)

The highest “nonorthogonality” \( |\Gamma_{mn}| \) appears when \( m = 12, n = 10 \) (or vice versa) in both cases, which are 0.1888 and 0.3934, respectively. Although the “nonorthogonality” \( |\Gamma_{mn}| \) between the adjacent odd or even \( E_i(r_0, \theta_0) \) may increase with a higher-order \( q \), given the actual nanofabrication tolerances, the PSWFs \( \psi_n(c, x) \) that we can use should be well limited to those with low correlation. Nevertheless, we can always use methods such as the Gram–Schmidt process to orthogonalize the bases \([32]\). These results suggest that with acceptable resolution, it is possible to fabricate subwavelength-sized metasurfaces that produce arbitrary wavefront with high conversion efficiency within the subwavelength propagation region.

If forming the structure requires fine elements that are too small to be fabricated, the scheme is of less interest. In what follows, we consider fabrication imperfection and give two explicit examples of the proposed subwavelength-sized metastructure designed to generate a subdiffraction hotspot in a desired direction within the subwavelength region. Consider using the first 13 discretized PSWFs \( \psi^N_n(c, x) \) to construct the metastructure.

\[ E_x(x_0, 0) = \begin{cases} \sum_{n=0}^{12} a_n \psi^N_n(c, x_0), & |x_0| \leq D/2 \\ 0, & |x_0| > D/2 \end{cases} \] (11)

where \( \psi^N_n(c, x) \) is the discrete equivalent of \( \psi_n(c, x) \). Let \( c = 0.5\pi \) and \( D = 0.5\lambda = 260 \text{ nm} \). Given that each \( \psi_n(c, x) \) has exactly \( n \) zeros in the interval \([-D/2, D/2]\), the number of the pixel \( N \) should be at least \( N_{\text{max}} + 1 \). Adjust the coefficient \( a_n \) to generate subwavelength concentration of light in a given position \( r' = (r', \theta') \).

Figure 3. Correlation matrixes of the vector propagation results of the first 13 order PSWFs at different radii, \( c = 0.5\pi, D = 0.5\lambda \). a) \( r_0 = 1\lambda \). b) \( r_0 = 0.75\lambda \).
Figure 4. Intensity propagation results, structure profiles, and the energy concentration ratio. a,b) Intensity propagation results and structure profile of a nanometagrating that generates a subwavelength hot spot at \( r' = (1\lambda, 0) \). The inset in (a) shows the profile of \( |E|^2 \) (the black dashed line), \( |E_x|^2 \) (the yellow solid line) and \( |E_z|^2 \) (the red dashed line) at the white dashed line. c–d) Intensity propagation results and structure profile of a nanometagrating that generates a subwavelength hot spot at \( r' = (1\lambda, \arcsin(0.97)) \). The inset in (c) shows the profile of \( |E|^2 \) (the black dashed line), \( |E_x|^2 \) (the yellow dashed line), and \( |E_z|^2 \) (the red solid line) at the white dashed line. For (b) and (d), the blue bars show the profiles of the absolute value of the amplitude of structure, and the purple needles show the profiles of phase. e) The energy concentration ratio \( \xi \) against \( N' = N/2(n + 1) \), where \( n = 12 \) is the highest order of the PSWFs used to construct the grating, \( c = 0.5\pi \), \( D = 0.5\lambda \). The solid line with uptriangle and the dashed line with right triangle represent the results in the cases of (a,b) and (c,d), respectively.
\[ a_n = \frac{i \cdot E_n^*(r', \theta')}{\sqrt{\int_{-\infty}^{\infty} \|E_n(r', \theta')\|^2 d \sin(\theta')}} \] 

where \( E_n(r, \theta) \) is vector propagation result of \( \psi_n(x, y) \), and \( E_n^*(r, \theta) \) is its conjugate function; \( i \) is the tangential unit vector at \( r' = (r', \theta') \). Let \( r' = 1 \lambda \). The calculated propagation results for \( \theta' = 0 \) and \( \theta' = \arcsin(0.97) \) are shown in Figure 4b,c. As can be seen the hotspots are generated at the given positions in both cases. In Figure 4a, the first dark ring (the first minimum) of the intensity of the tangential component \( |E_n|^2 \) appears at \( x_1 \approx 0.33 \lambda \), and the first inflection point of the total intensity \( \|E\|^2 \) appears at \( x_1 \approx 0.35 \lambda \). In the second case, the full width at half maximum of \( |E_n|^2 \) and \( \|E\|^2 \) are approximately 0.35 and 0.40\( \lambda \), respectively. The corresponding structure profiles are given in Figure 4b,d. Given that \( N = 26 \) and \( D = 0.5 \lambda = 260 \text{nm} \), the width of the finest structure of the grating \( d = 10 \text{nm} \), which is totally possible to be fabricated by current nanotechnology. The ability of the structure to tolerate manufacturing imperfection is related to the intrinsic noise relaxation mechanism of subwavelength structures, which suggests that the propagation results of the fine deep-subwavelength structure with no zeros tend to the result of a point-spread function with which the source amplitude equals the average complex amplitude of the fine structure. The earlier results suggest that within the range of acceptable manufacturing tolerance, the proposed nanometagratings can generate arbitrary complex sub-diffraction patterns in subwavelength diffraction regions, with subdiffraction resolution.

As the undesired sidelobes are apodized, the energy transformation efficiency of the proposed metagratings is in principle unitary. Here we define a parameter \( \xi \) as the ratio between the energy concentrated in a given angle \( (\theta_1, \theta_2) \) and the total energy in the whole range \((-\pi/2, \pi/2)\) to further characterize the energy concentration ability of the proposed metagratings when fabrication imperfection exists. For the first case in Figure 4, we choose the interval to be \( \theta_1 = \theta_2 = \arctan(D/2r') \), which gives \( \xi \approx 0.66 \).

For the second case, we choose \( \theta_1 = \arctan(r'/2D), \theta_2 = \pi/2, \) and \( \xi \approx 0.82 \). The reason for the general difference in \( \xi \) in the two cases is that in the first case, a small portion of the energy is dispersed to the proximity \( |\theta| \approx \pi/2 \), as indicated by Figure 2f (see the red solid line). Even though, due to the apodization of the strong sidelobes, these ratios are at least several orders of magnitude higher than that of traditional superoscillations lenses with similar resolution. These ratios \( \xi \) will increase with the number of the pixels \( N \) in both cases, as clearly shown in Figure 4e. For example, in the first case when \( N/2(n+1) = 2 \), \( \xi \) soon reaches 0.69, and the corresponding width of the pixel is 5 nm when we still choose \( \lambda \) to be 520 nm. Moreover, the energy ratio \( \xi \) will further increase when more PSWFs are used. For example, when \( n = 14 \), \( N/2(n+1) = 2 \), \( \xi \) reaches to \( \approx 0.73 \), and the corresponding pixel size is \( \approx 4.33 \text{nm} \). These results suggest that the energy concentration ability of the proposed metastructure is much higher than the traditional superoscillations device, and it will be further improved by finer production; however, a wider period with less pixels will relax the fabrication requirement at the expense of lower resolutions and lower \( \xi \). More results illustrating the role of manufacturing imperfection are given in Figure 5 in Supporting Information II.

We believe that nanometagratings promise a vast variety of novel applications. Given the previous works achieving quantum information processing with the conventional large-scale optics, here, we discuss one of the application scenarios, that is to use the nano metagratings to build a “nanophoton gate” to achieve optical quantum information processing in subwavelength scale. As depicted in Figure 5, the nanometagratings project the incident photons into two or more directions within subwavelength radius, each with different complex amplitude. If we regard each direction of propagation (or each path of propagation) as a quantum state, then we can obtain quantum gates with different functions by combining these nanometagratings. Figure 5 gives an example. We assume that a photon, after passing through a series of previous light paths, can only

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**Figure 5.** A Hadamard gate as the combination of two nanometagratings. The scale bar fits when \( D \approx 0.5\lambda \approx 0.25 \mu m \).
propagate to the right through gate 1 or upward through gate 2 and regard the two propagation modes of the photon as state $|1\rangle$ and state $|0\rangle$, respectively. Suppose the state of the photon before passing through the gates is

$$
\varphi = \alpha|1\rangle + \beta|0\rangle
$$

(13)

After passing through the photon gates, the state becomes

$$
\varphi = \frac{1}{\sqrt{2}}[(\alpha + \beta)|1\rangle + (\alpha - \beta)|0\rangle]
$$

(14)

In this way, we form a Hadamard gate with two proposed nanomemetagratings, which is but one of the most important quantum gates in the field of quantum computing. Similar approaches can be extended to achieve quantum gates with other functions. We believe that by proper design, a more complex highly integrated quantum computation photonics circuit can be realized.

3. Conclusion

In summary, we propose the theory of extreme subdiffraction photon control and point out new physical mechanisms enabling rational designs for general highly efficient nanosized metasurfaces, which cannot be reasoned by current propagation theories. We demonstrate a new class of novel metasurfaces named “nanometagratings”, which are planar metasurfaces that are smaller than one wavelength, and manage to achieve arbitrary wavefront engineering with near-unitary efficiency, enabling extreme photon control within subwavelength scale. We demonstrated that the structure can be formed by an array of finite elements not exceeding the current fabrication limitations, and discuss one of the application scenarios, that is to use these nanometagratings to build a “nanophoton gate” to achieve optical quantum information processing in subwavelength scale. Our results are expected to open the era of ultrasmall highly efficient metasurfaces and promise novel applications such as highly integrated photon computation.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

Research data are not shared.

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