Deep-subwavelength gap modes in all-dielectric metasurfaces for high-efficiency and large-angle wavefront bending

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**Abstract:** All-dielectric, phase-gradient metasurfaces manipulate light via a judiciously designed planar distribution of high and low refractive indices. In the established design approaches, the high-index elements play a dominant role, while the electromagnetic field existing between these elements is routinely viewed as either an incidental by-product or detrimental crosstalk. Here we propose an alternative approach that concentrates on exploring the low-index materials for wavefront shaping. In our Si metasurface, the low-index air gap between adjacent Si fins is judiciously tuned, while the high-index Si fins only have a single size across the whole metasurface. These gap modes provide the full 2π phase coverage, as well as high and relatively uniform transmission, at the deep-subwavelength scale. These characteristics are ideal for mapping a steep phase gradient, consequently suitable for high-efficiency and large-angle wavefront bending. This light manipulation capability is exemplified with numerical simulation in PW-SW (freely propagating wave to surface wave) conversion, where the wavefront is deflected by an angle of 90°. In the gap-mode meta-converters, the average unit size can be only 1/60 of free-space wavelength, an order of magnitude smaller than that of conventional all-dielectric metasurfaces. Their conversion efficiency can reach 68%, the highest value reported for any all-dielectric gradient metasurface THz converter.

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1. Introduction

Deflecting incident light at large angles and high efficiencies using nano- and microstructures promises various applications in spectroscopy [1], imaging [2], optical holography [3], sensing [4] and on-chip photonic circuitry [5]. Recently, all-dielectric metasurfaces [6,7] have emerged as a promising new approach to this goal. In addition to their capability of providing a high level of wavefront control, these metasurfaces are inherently low in optical loss [8-10], which is widely regarded as an important advantage over metallic metasurfaces in regimes from the terahertz (THz) to the visible. However, for large-angle wavefront bending, in particular in the form of PW-SW (freely propagating wave to surface wave) conversion, their performances are actually far inferior to those of plasmonic and metallic metasurfaces [11-14]. As compared to the nearly perfect PW-SW conversion reported in metallic metasurfaces, the conversion efficiency is much lower in all-dielectric, phase-gradient metasurfaces. The record value that we can find is only 39.5%, according to the numerical simulation of Ref. [15].

Large-angle, high-efficiency wavefront bending is a challenging task for all-dielectric, phase gradient metasurfaces, mainly due to these two limiting factors: relatively large transversal size of dielectric elements [16], and the finite crosstalk between adjacent elements. For an all-dielectric, phase-gradient metasurface to change the propagation direction of linearly polarized incident light while preserving its polarization direction, as required in the majority of applications, two design approaches are widely adopted in the research community [17-19]. The first utilizes the Mie resonance, and the second is based on the effective refractive index approximation. The Mie resonance approach provides the required 2π phase coverage by overlapping electric and magnetic dipolar Mie-type resonances of a high-index dielectric resonator [17]. As both resonances are highly sensitive to the size and the aspect ratio of the resonator, the planar dimensions of the resonator cannot be significantly smaller than the free-space wavelength λ0 of the incident light. For example, in circular Si pillars residing on a glass substrate, regarding the side length of a light scattering unit, a guideline value is λ0/2 [8, 20, 21]. Here a unit refers to a section of a metasurface that consists of both high and low index materials, and several similar or equal-sized units form a super unit cell, which is the smallest periodic part of a metasurface. For the second approach that utilizes the effective refractive index approximation, the phase accumulation is proportional to the metasurface thickness for a given planar pattern [19, 22]. This feature consequently allows for a more compact in-plane unit distribution, where the unit side length typically ranges from λ0/2 to λ0/5 [15, 22-25]. Further reducing the unit size is apparently unfeasible based on existing reports. In the conventional view [26], it is mainly due to the crosstalk between adjacent high-index units.

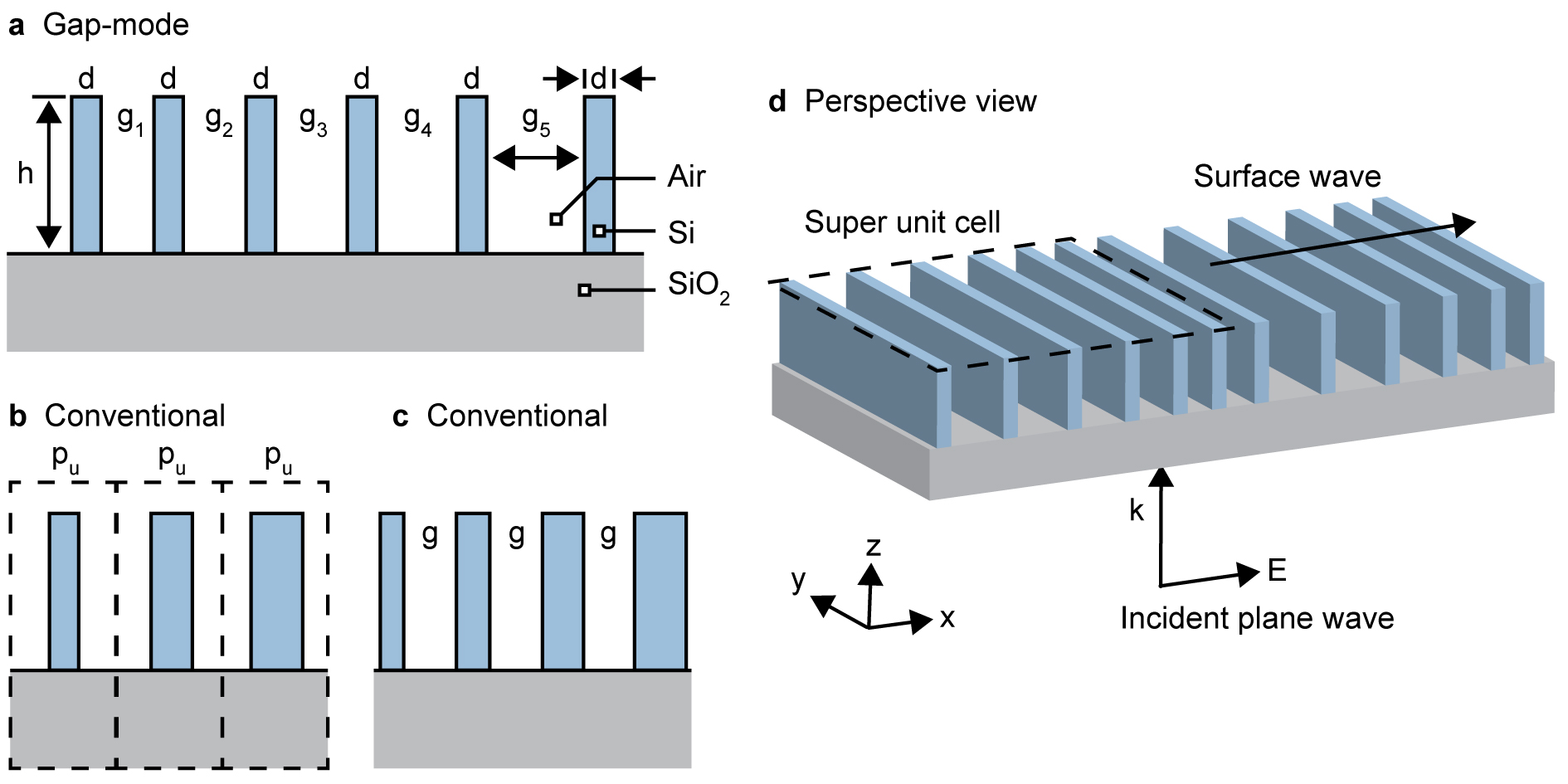
In all-dielectric metasurfaces, crosstalk appears as a strong electromagnetic field existing between adjacent elements of high-index materials. The magnitude of the crosstalk depends on the gap size between high-index elements, as well as light deflection angle. As pointed out in Refs. [16, 22, 27] for the second design approach discussed above, the influence of crosstalk frequently hinders wavefront bending for any angle larger than ~40°. By comparison, for the PW-SW conversion under normal incidence, the target application analyzed here, the deflection angle is required to be 90°. It is worth pointing out here a recent work [28], which utilizes a metasurface to convert a PW to a waveguide mode in the near-infrared regime. Because of the total internal reflection inside the waveguide, the PW and the guided mode form an acute angle in their propagating directions, effectively reducing the light deflection angle for the metasurface. By comparison, the SW discussed here propagates along a direction orthogonal to that of the incident wave, and its excitation requires wavefront bending at exactly 90°.

In this work, we propose a new design strategy that is dedicated to high-efficiency, large-angle wavefront bending. Rather than trying to suppress or eliminate the influence of the electromagnetic field between adjacent high-index elements, this work adopts an opposite approach, by judiciously exploring it for light bending. The contrast between this new approach and the two established approaches discussed above can find some analogy in Si photonics research. While the electromagnetic field at the waveguide surface is considered a source of loss in rib and ridge waveguides, this field is utilized in slot waveguides for sensing [29, 30]. We show here that the same principle can also be applied in all-dielectric metasurface research: the field between the gaps of high-index materials can be functional rather than detrimental.

In the following sections, we concentrate on demonstrating SW excitation in these gap-mode metasurfaces in the THz regime. Multiple PW-SW THz meta-convertors have been reported [31-36], with target applications ranging from light focusing [31] and sensing [32, 33, 36] to on-chip THz systems [34]. A high conversion efficiency is critical for all these potential applications, and this work shows that it can be achieved using gap-mode dielectric metasurfaces.

1. Si metasurfaces and their gap-mode configuration

Figure 1 schematically illustrates three Si metasurfaces, with a gap-mode Si metasurface [Fig. 1(a)] shown in comparison to two conventional Si metasurfaces [Figs. 1(b) and 1(c)]. All the three metasurfaces are a one-dimensional grating of Si fins that are infinitely long along the planar *y* axis. In the gap-mode metasurface [Fig. 1(a)], all the Si fins are identical, while the air gap varies in width across a super unit cell. In contrast, a conventional design usually adjusts the width of both the fin and the gap [Fig. 1(b)], or only that of the fin [Fig. 1(c)]. Although this difference may seem subtle, Fig. 1(a) in fact reveals a new design strategy for all-dielectric, phase-gradient metasurfaces.



**Fig. 1.** Schematic of three different types of phase-gradient metasurfaces. All the metasurfaces consist of a one-dimensional grating of infinitely long Si fins residing on top of a glass substrate. (a) The gap-mode metasurface proposed in this work produces a designated phase gradient only by tuning the air gap width (from to in the schematic). All the Si fins have an identical width of . (b) A conventional design strategy would require a uniform unit periodicity , which is equivalent to a uniform center-to-center distance between adjacent high-index elements. This results in variations in both and across a super unit cell. (c) Another conventional design strategy would require the gap width to be a constant. (d) A perspective view of the gap-mode metasurface for PW-SW conversion. The metasurface is illuminated by a plane wave at normal incidence from the glass substrate. The free-space wavelength λ0 is 375 μm, and the light is linearly polarized in the *x* direction. A super unit cell, which is the smallest periodic unit, is highlighted using the dashed parallelogram.

To clarify the contrast of these three designs and the underlying design strategies, Fig. 2 shows the numerically simulated electromagnetic properties of a set of constituent units. Here a unit is a Si fin with air gaps on its two sides, or alternatively an air gap with Si fins on its two sides. The simulation, for Fig. 2 and all that followed, was conducted using a commercial finite element solver (COMSOL Multiphysics). The simulation covered both periodic and non-periodic structures, for which the settings followed our recent works [20, 37]. The glass substrate, which mechanically supported the Si fins, was treated to have an infinite thickness. The incident light had a frequency of 0.8 THz and a free-space wavelength λ0 of 375 μm. It illuminated the Si fins at normal incidence from the glass side, and had a polarization orthogonal to the fins (i.e. along the *x* axis in Fig. 1). Both Si and SiO2 were treated as lossless, and their dielectric constants [38, 39] were 11.67 and 3.84, respectively.

Figures 2(a) and 2(b) show the dependence of light transmission on the gap size and the fin width , with the fin height fixed at 600 μm. The results possess these two features that are crucial for constructing phase-gradient metasurfaces: the full 2π coverage in the output phase [Fig. 2(a)] and the mostly stable output intensity [Fig. 2(b)]. Figure 2(a) shows that the 2π phase coverage, a prerequisite for full wavefront control, can be achieved in deep-subwavelength regions. For example, it exists in the area where both and are between 5 μm and 25 μm, with the upper boundary merely λ0/15. Figure 2(b) further shows that the intensity variation is relatively small in the deep-subwavelength regime. For example, in the same area of , the variation range is within 0.87 and 1.00 (perfect transmission). These two features suggest that, the unit library shown in Figs. 2(a) and 2(b) can map a target phase profile at high fidelity, even if the profile is highly position dependent (e.g. a steep linear ramp).

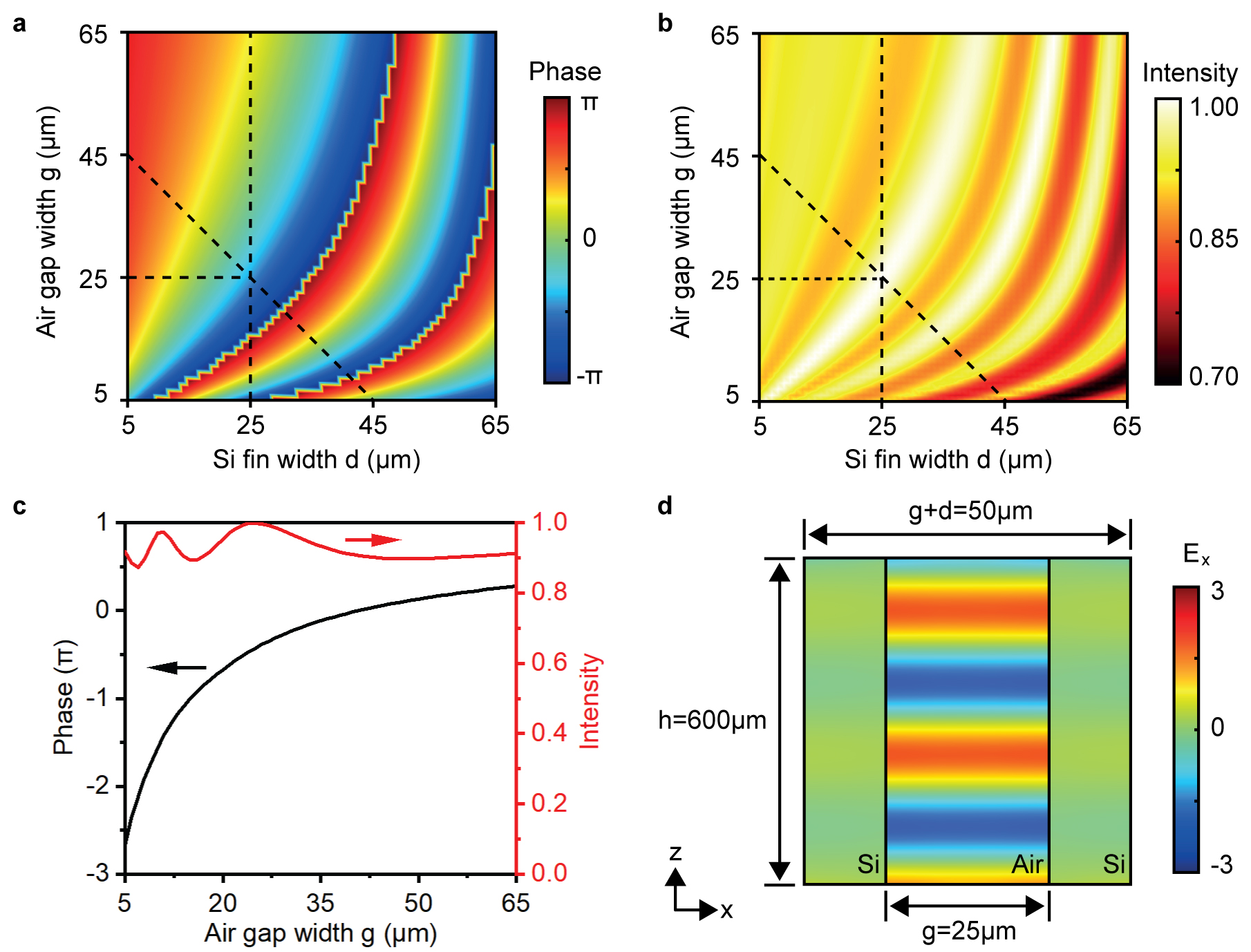


Fig. 2. Relative phase and intensity of light transmission for a range of gap-fin units. (a) The air gap width and the Si fin width are tuned independently from each other, in the same range from 5 μm to 65 μm. The phase is with respect to the incident light. The three dashed lines converge at , a representative point that is chosen to facilitate discussion. (b) The intensity of the transmitted light with respect to the incident light, for the same dimensional range. (c) The variation in the phase and the intensity, with fixed at 25 μm (i.e. 1/15 of the free-space wavelength λ0) and tuned across the whole range. The data corresponds to the vertical lines in (a) and (b). (d) Electric field distribution insides a representative unit, normalized against the incident light inside the SiO2 substrate. It has , corresponding to the point of line convergence in (a) and (b). The electric field inside the air gap is enhanced by a factor of 2.4 as compared to the incident field. In all the four panels, the fin height is set as 600 μm, a parameter that is analyzed in following discussions and adjusted in other examples.

We now consider a task of picking a few elements from the library in Figs. 2(a) and 2(b) to provide uniform phase coverage of 2π. A conventional solution, which corresponds to the metasurface in Fig. 1(b), is to pick elements from a line parallel to the diagonal line in Figs. 2(a) and 2(b). This solution guarantees that is a constant for all the units in a super unit cell. Another solution is to pick elements from a horizontal line, where is a constant in a super unit cell. These two solutions correspond to metasurface design strategies that generate a uniform unit cell size and a uniform gap size. Example metasurfaces following these two design strategies can be found in Refs. [15, 40].

A key claim of this work is that, there exists a third solution, which is to pick elements from a vertical line in Figs. 2(a) and 2(b). In this solution, rather than is a constant. It implies that, all the Si fins in the metasurface have an identical size, as drawn schematically in Fig. 1(a). Here the designated phase profile is generated purely by placing these identical fins at varying intervals. As a numerical demonstration, Fig. 2(c) shows the output phase and intensity at an example fin width of . A phase coverage of 1.48×2π is observed in the whole simulated range of , and the intensity is always above 0.87. Figure 2(d) shows the electric field distribution of a representative unit, with has . The field almost exclusively resides within the air gap, which can be referred to as an electromagnetic gap mode.

We would like to highlight that this gap-mode solution represents an interesting new design strategy. Although gap modes have been intensively studied in plasmonic metasurfaces [41], their counterparts in all-dielectric metasurfaces are rarely discussed [42-45]. In the majority of previous works on all-dielectric metasurface, the material with a high refractive index is viewed as being functional, and it attracts most of the research effort in analyzing metasurface properties. In this new design strategy, as demonstrated in Fig. 1(a) and Fig. 2, all the Si fins have an identical shape (i.e. an identical ). Consequently, the opposite viewpoint is more natural: the low-index material (here air) is judiciously tuned, while the high-index material (here Si) is the uniform background. A target phase gradient is achieved by separating identical high-index elements at designated, variable low-index gaps. To the best of our knowledge, the possibility of this strategy has never been discussed before, either in a one-dimensional metasurface (the category of the metasurfaces analyzed here) or in a two-dimensional metasurface.

In the following discussion, we first provide in Section 3 analytical interpretation of the results in Fig. 2. The interpretation not only provides insight into these results but also helps determine the value of fin height, which is chosen arbitrarily for Fig. 2. In Section 4, we analyze several gap-mode metasurfaces for PW-SW conversion, which serve as a numerical implementation of the design strategy in high-efficiency and large-angle light bending.

1. Transfer matrix analysis

We interpret the results shown in Figs. 2(a) and 2(b) by first making a comparison with the conventional design approach that is based on the effective refractive index approximation. In the effective index approach, the phase accumulation for light λ0 passing through a metasurface unit with thickness is expressed as , where is the effective refractive index. This equation is derived from a single pass of the incident light in the film, and it ignores the multiple reflection of light inside the film. Here, for analyzing the gap-mode metasurfaces, we take the multiple reflection into consideration, which is achieved by using the transfer matrix analysis.

As every point in Figs. 2(a) and 2(b) corresponds to an infinitely large, periodic array of air slits in a Si film, we first extract the values of for such films. These values are obtained in numerical simulation from mode analysis [Fig. 3(a)], where and are tuned independently from each other in the same range as in Figs. 2(a) and 2(b). A pronounced feature of Fig. 3(a) is the monotonic increase in from the top left to the bottom right. The top left corner corresponds to wide air slits (65 μm) separated by narrow Si fins (5 μm), and the value of is 1.04, close to that of air. By comparison, the bottom right corner corresponds to narrow air slits (5 μm) separated by wide Si fins (65 μm), and is 2.82, much closer to that of Si. More discussion on the mode analysis can be found in Supplementary Fig. S1.



**Fig. 3.** Transfer matrix analysis for the constituent units of gap-mode metasurfaces. (a) The effective refractive index of the gap mode, obtained by assuming an infinitely large film thickness . The fin width and the gap width vary from 5 μm to 65 μm. (b) The output phase and (c) the output intensity from the gap modes. In both (b) and (c), the film thickness is 600 μm, the same as that in Fig. 2. (d) The phase coverage achievable at four representative values of (10 μm, 15 μm, 30 μm and 45 μm), as ranges from 100 μm to 800 μm. Each data point is obtained by scanning from 5 μm to 65 μm. The solid lines utilize the transfer matrix analysis, and the dots are purely from numerical simulation.

From the values of , we can obtain the complex transmission coefficient for any film thickness , by using the transfer matrix analysis. The transfer matrix is a 2×2 matrix [46, 47] expressed as

where is the imaginary unit and is the phase shift in the film. The transmission coefficient and the reflection coefficient can be expressed respectively as

where and are the refractive index of the substrate (SiO2) and air, respectively. For each pair of and , the coefficients and are computed using the results in Fig. 3(a) and the three equations above. The transmission phase and transmission intensity [here utilizing the lossless feature of the device] are shown in Figs. 3(b) and 3(c), respectively. The results match well with those in Figs. 2(a) and 2(b), which are obtained from pure numerical simulation (see Supplementary Fig. S2 for details). This close matching indicates that the gap mode discussed here can be treated as an effective medium, given that multiple reflection inside the medium is considered.

Before analyzing any specific gap-mode metasurface, it is worth discussing a key parameter here, the phase coverage. It is well accepted that a unit library, or a subset of it, needs to provide the complete 2π phase coverage, in order to enable a high level of wavefront control in the resulted metasurfaces. As a gap-mode metasurface is required to have a uniform fin width , the phase coverage depends on the other two geometric parameters, the fin height and the gap size . Figure 2(d) shows the influence of on the total phase coverage of Δφ, by limiting the range of to 5 μm ~ 65 μm (i.e. the same range used in Fig. 2 and the other panels of Fig. 3). Both the pure numerical method, which is implemented for Fig. 2, and the numerical-analytical hybrid method, which is implemented for Figs. 3(b) and 3(c), are tested here, and they produce almost identical results. The results show that, if the Si fins decrease in width , they have to increase in height to provide the 2π phase coverage. For example, at , can be any value above 362 μm. Once reduces to 10 μm, the 2π threshold of increases to 695 μm. This result is used for the analysis in Section 4.

1. SW meta-couplers based on gap-mode metasurfaces

Due to their unique characteristics of deep-subwavelength feature sizes, full 2π phase coverage and relatively small output intensity fluctuation, these gap modes are ideal for creating a steep phase gradient. In this section, we exemplify these characteristics with the numerical demonstration of PW-SW conversion. At normal incidence shown in Fig. 1, the bending in the wave propagation direction is 90o, which is a challenge for many metasurface designs [16, 22, 27].

Following the steps taken in our recent work on stretchable PW-SW meta-converters [37], we first analyze in Fig. 4 the configuration where an infinitely large meta-converter (or a meta-coupler) is uniformly illuminated by a plane wave. The configuration is then modified to approximate future experiments in Fig. 5, where only a limited area on the meta-converter is illuminated. This procedure of analysis can provide a clear visualization of the SW (in Fig. 4), as well a conversion efficiency (in Fig. 5) that is comparatively easy to verify in future experiments.

To demonstrate the flexibility in the gap-mode metasurface design, Fig. 4 presents four different meta-converters, where the unit number (i.e. the number of gaps) in a super unit cell is 8, 16, 30 and 60 in Figs. 4(a)-(d), respectively. In all the four designs, the periodicity (, the dimension of a super unit cell in the planar direction orthogonal to the fins) is slightly smaller than the free-space wavelength λ0 of 375 μm, in order to eliminate any diffraction order into free space [11, 37]. Its exact value is 367.0 μm, 371.5 μm, 367.0 μm and 369.3 μm from Figs. 4(a) to 4(d). Due to this almost invariant value of , an increase in unit number from 8 to 60 in a super unit cell consequently requires a significant decrease in the fin width . Based on the results in Fig. 3(d), the height consequently has to increase from Figs. 4(a) to 4(d). After several rounds of numerical optimization, the value of settles at 425 μm, 710 μm, 830 μm and 950 μm in Figs. 4(a)-(d), respectively. The output phase and intensity of all the units in these four designs, together with their geometric dimensions, can be found in Supplementary Fig. S3 and Table S1.

Figure 4 shows that all the four designs support a strong SW at the top surface (i.e. the *xy* interface between the Si fins and the air) of the meta-converter. The SW decays exponentially into the air along the *z* axis at a rate of in all the designs, where the characteristic depth is design dependent and varies between 270 μm to 380 μm. Meanwhile, the *z*-direction decay inside the meta-converter lacks such exponential dependence. This is attributed to the spatial variation in the refractive index inside the meta-converter, as well as the existence of a weak Fabry–Pérot resonance between its two *xy* surfaces. The latter is most noticeable in Fig. 4(a), where an oscillation of the strength of the component is visible along the *z* axis inside the meta-converter.



**Fig. 4.** PW-SW conversion in four infinitely large, periodic meta-couplers. The periodicity is approximately 370 μm in all the four designs. Each panel corresponds to an area of 1850 μm ×1500 μm, each containing 5 super unit cells. The meta-converters are illuminated at normal incidence from the bottom by a linearly polarized PW. The polarization is along the *x* axis, which is orthogonal to the Si fins. The field strength of all the four panels is normalized against the same value. The number of air gaps in a super unit cell is (a) 8, (b) 16, (c) 30 and (d) 60. Panels (a) and (d) are annotated for clarification, and the hatched areas in all the panels specify the spatial expansion of a single super unit cell.

In all the four designs in Fig. 4, the SW propagates in the +*x* direction, the direction of decreasing gap size inside a unit cell. The propagation constant is equal to the phase gradient as shown below

where is the wavelength of the SW. The second equality of the equation originates from the fact that follows the periodicity . As is slightly smaller than λ0, is slightly larger than the free-space propagation constant of the incident light. The bandwidth of both devices is further discussed in Supplementary Figs. S4 and S5. Based on the shape and intensity of the output wave, the functional wavelength range has a span of approximately 25 μm and 15 μm for the 8- and 60-unit devices, respectively. Within the bandwidth range, the SW wavelength always equals the periodicity .

To better approximate future experiment and to enable efficiency calculation in the PW-SW conversion [11-14, 37], two of the four designs studied above are further analyzed in Fig. 5. Following previous works, including one from our team [37], the input light is restricted in its width, and the output SW is converted to a self-sustained guided wave for efficiency analysis. In both panels of Fig. 5, the SW is coupled into a 105 μm thick glass slab placed in the vicinity of the meta-converter. The incident plane wave has a limited width, illuminating only a single super unit cell. Both designs shown in Fig. 5 produce a strong guided wave in the glass slab. Further analysis on the strength of the guided wave leads to a PW-SW conversion efficiency in the 8-unit meta-converter [Fig. 5(a)] of 66.6%. The efficiency is slightly higher in the 60-unit meta-converter [Fig. 5(b)], reaching 68.3%. This value represents a relative increase of ~70%, and an absolute efficiency increase of ~29%, from the current record in all-dielectric PW-SW gradient converters [15]. It is worth highlighting here that, the average unit width of this design is only λ0/60, at a truly deep-subwavelength scale.



**Fig. 5.** PW-SW conversion in two finite-sized meta-couplers. Both couplers contain only a single super unit cell. The incident plane wave has the same width as the super unit cell and it is launched at 500 μm beneath the Si-SiO2 interface. The unit number in a single super unit cell is (a) 8 and (b) 60. The arrows indicate the wave propagation directions.

To further increase the conversion efficiency in the future, these two main sources of loss need to be addressed: light reflection and metasurface-glass slab coupling. The reflection occurs at both the Si-air and the Si-SiO2 interfaces, and it directs energy back to the SiO2 substrate. Although it is an inherent property of the meta-converter, its magnitude can be suppressed by optimizing the fin height or adopting multi-layered fins. By comparison, the metasurface-glass slab coupling is not an inherent feature of the meta-converter. Such kind of coupling is necessary, as the SW is a driven mode and it has to be transformed into an eigenmode for future utilization. As the PW-SW conversion efficiency is computed based on the energy of the eigenmode, the glass slab thickness used in Fig. 5 has been optimized to achieve an effective transformation from the driven mode to the eigenmode at 375 μm. The glass slab used here follows recent experimental works [13], and its eigenmode is a confined waveguide mode. It is also possible to convert the driven SW to other types of eigenmodes, e.g. surface plasmons [14]. The PW-SW conversion efficiency also depends on the number of super unit cells [14, 48], which is analyzed in Supplementary Fig. S6.

Before concluding this work, it is worth discussing briefly the microfabrication of these designs in future experiments. As a proof-of-principle demonstration of the all-dielectric gap modes, the analysis above has been conducted without considering any microfabrication constraint. A major constraint that is often encountered in experiment is the aspect ratio [49-51], which, for the designs discussed above, set a lower boundary on for a given set of and . To benefit future experiment, the maximal aspect ratios of a few meta-converter designs are listed in Supplementary Table S1, in addition to all their geometric parameters. These devices could be fabricated by applying deep reactive ion etching on a Si film, following fabrication processes detailed in several references [49-51]. Taking 160 as the maximal aspect ratio achievable in experiment [49], we envisage that meta-couplers with a unit number of 8, 10, 12 and 16 (i.e. the first four designs listed in Table S1) can be obtained using this ion etching technique.

1. Conclusion

To conclude, we have proposed and numerically tested a new design strategy for all-dielectric metasurfaces that exploits the electromagnetic responses of low-index materials. One-dimensional gratings of Si fins are used for analysis, where all the Si fins are identical in a metasurface. Adjusting the deep-subwavelength air gaps between adjacent fins provides not only the full 2π phase coverage but also high and relatively uniform output intensity in transmission. These characteristics allow for accurate mapping of a steep phase profile, as required for scenarios such as high-efficiency, large-angle wavefront bending. Several THz meta-converters are analyzed to demonstrate this wavefront manipulation capability. The conversion efficiency can reach 68%, the highest value reported in all-dielectric, phase-gradient THz converters.

It is worth pointing out that to utilize this new gap mode, it is not a prerequisite to force all the high-index elements to have an identical shape and size. We choose to have an identical Si fin width in our discussions, because it can explicitly reveal the role of the air gap. A generalized gap-mode all-dielectric metasurface instead can have variable dimensions for both the high- and the low-index elements. Different unit selection methods [52, 53], for example the inverse design method [54], could be applied on the gap modes to achieve different functionalities.

This work has demonstrated that the gap modes, which could be perceived as a useless by-product or even detrimental crosstalk in existing design strategies, can be utilized to achieve light manipulation that is extremely challenging for existing strategies. Besides the PW-SW conversion analyzed here, these gap modes can be used in many other applications that benefit from high-efficiency, large-angle wavefront bending, further expanding the application realm of all-dielectric metasurfaces.

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**Data availability.** Data underlying the results presented in this paper are not publicly available at this time but may be obtained from the authors upon reasonable request.

**Supplemental document.** See Supplement 1 for supporting content.

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