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# Antireflection of optical anisotropic dielectric metasurfaces

Yu-Hsuan Liao, Wei-Lun Hsu, Chen-Yi Yu & Chih-Ming Wang

We propose a hetero-nano-fin structure to further improve the efficiency of Pancharatnam–Berry phase metasurfaces. Two hetero-nano-fin types,  $\text{MgF}_2/\text{GaN}$  and  $\text{MgF}_2/\text{Nb}_2\text{O}_5$ , were investigated. The overall polarization conversion efficiency (PCE) improved from 52.7 to 54% for the  $\text{MgF}_2/\text{GaN}$  nano-fin compared with the bare GaN nano-fin. The overall PCE of the  $\text{Nb}_2\text{O}_5$  nano-fin was 1.7 times higher than that of the GaN nano-fin. The overall PCE improved from 92.4% up to 96% after the application of  $\text{MgF}_2$  antireflection. Moreover, the antireflection improves efficiency by an average of 4.3% in wavelengths from 450 to 700 nm. Although the increment of energy seems minimal, antireflection is crucial for a metasurface, not only enhancing efficiency but also reducing background signal of a meta-device.

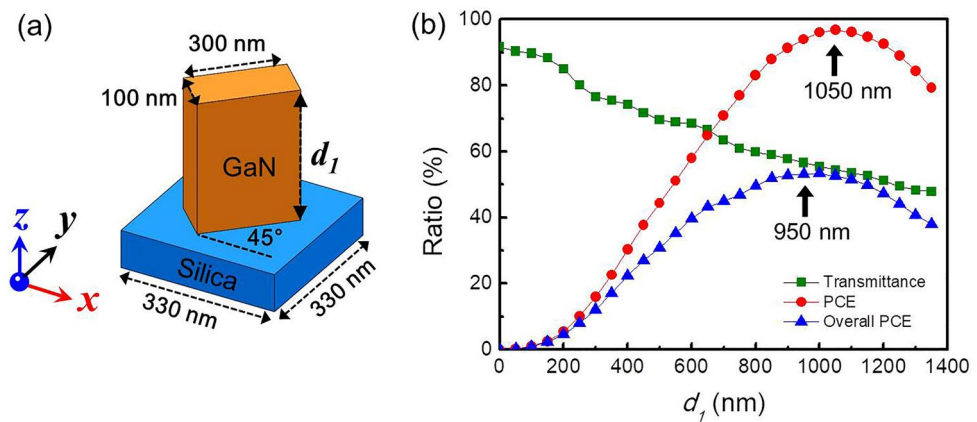
Plasmonic metasurfaces, consisting of two-dimensional metallic meta-atom arrays, are advantageous because of their properties such as ultrathin thicknesses, ease of fabrication, versatile functionality, field confinement beyond the diffraction limit, and superior nonlinearity<sup>1–6</sup>. Although a plasmonic metasurface has an impressive light modulation ability, its efficiency is limited as it suffers from Ohmic heat loss during resonance. Huygens meta-atoms, which are meta-atoms in which resonances of the electric dipole and magnetic dipole coincide, can break the scattering symmetry and improve the transmission efficiency<sup>7,8</sup>. Although zero back-scattering can be achieved under the first Kerker condition<sup>9</sup>, the transmission efficiency of a plasmonic metasurface is limited at a visible frequency.

A dielectric metasurface almost effortlessly avoids Ohmic heat loss and has therefore rapidly attracted extensive research attention. In addition to resonance-based light modulation, the dielectric metasurface is generally capable of two typical light modulation methods: propagation phase<sup>10–14</sup> and geometric phase<sup>15–21</sup>. The propagation phase involves phase accumulation during light propagation. For a fixed propagation path, the effective index of the metasurface determines the optical path difference (OPD), such as controlling the filling ratio of the material. The geometric phase is also termed the Pancharatnam–Berry (PB) phase. Light carries an additional phase when it passes through an optical anisotropic structure/material. Spatially varying geometric orientation of the optical anisotropic structure can control phase distribution. Moreover, the original polarization state of light changes to the orthogonal one (e.g., left-hand circular polarization to right-hand circular polarization) and carries geometric phase modulation. Therefore, the PB-phase metasurface also acts as a half-waveplate for polarization conversion. However, the half-waveplate condition does not coincide with the antireflection condition. Moreover, materials with a high refractive index are suitable as dielectric metasurfaces; however, they usually lead to impedance mismatch at the interface. Consequently, the PB-phase metasurface suffers from severe Fresnel reflection loss.

A traditional antireflective thin-film consists of single or multiple homogeneous layers and has refractive indices and thicknesses suitable for reducing the Fresnel reflection at the interface. Sub-wavelength structures, such as gratings<sup>22</sup>, pillars<sup>23,24</sup>, pyramids<sup>25,26</sup>, moth-eyes<sup>27–29</sup>, and nanopores<sup>30</sup>, may also be used for antireflection. These structures generate a gradient effective refractive index to reduce the refractive index contrast between air and the medium through which light is entering. Nowadays, sub-wavelength structure-based antireflection has been widely used for photovoltaic solar cells<sup>31–36</sup>.

Macroscopically, a dielectric PB-phase metasurface is an optically anisotropic medium that is similar to a birefringent structure. In 2001, Mohammed et al. applied an antireflection coating on smooth surfaces by exploiting the anisotropic nano-topology of a liquid-crystal polymer film<sup>37</sup>. In 2018, Zhu used three laminating layers as a broadband antireflection coating for a birefringent sapphire waveplate<sup>38</sup>. The aforementioned studies investigated reflection from a homogeneous and anisotropic layer. However, microscopically, as the dimension of meta-atoms is close to the incident light wavelength, the metasurface should be considered an inhomogeneous, but not a homogeneous, anisotropic medium.

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**Figure 1.** Geometric diagram and optical property of GaN nano-fin. **(a)** Geometric diagram of a GaN nano-fin on a silica substrate, where  $d_1$  is the thickness of the nano-fin. **(b)** Transmittance, PCE, and overall PCE versus the thickness of the nano-fin under light illumination of 633 nm at normal incidence along the  $z$ -direction from bottom to up. The polarized light is along the  $x$ -direction. The light is  $x$ -polarized, with  $\lambda = 633$  nm. The light impinges perpendicularly onto the structure from bottom along the positive  $z$ -direction.

In this work, we investigated the antireflection layer for the PB-phase metasurface. First, we discussed whether the traditional antireflection layer is suitable for the dielectric PB-phase metasurface. Then, an antireflection structure was proposed to enhance the efficiency of the metasurface. We then numerically investigated the overall polarization conversion efficiency (PCE) and optical properties of both gallium nitride (GaN) and niobium oxide ( $\text{Nb}_2\text{O}_5$ ) nano-fins with an antireflection structure. To obtain the highest PCE, the thickness of the nano-fin was corresponded to a half-waveplate. Magnesium fluoride ( $\text{MgF}_2$ ), a common low-index material for antireflection, was chosen as the antireflection layer. Here, we simulated the overall PCE enhancement and optical properties with three different arrangements of the  $\text{MgF}_2$  layer. Based on the calculated results, an antireflection structure for the dielectric PB-phase metasurface was proposed. Thus, antireflection for the metasurface is crucial for enhancing the efficiency as well as reducing the background signal of a meta-device.

## Results and discussions

As shown in Fig. 1a, the basic building block is a GaN nano-fin on a silica substrate. The nano-fin had its basic dimensions fixed (length: 300 nm, width: 100 nm, and period: 330 nm), while its thickness ( $d_1$ ) was varied for the analysis of corresponding optical properties. All simulations were performed using the finite-difference time domain method, which is used to simulate the PCE and transmittance. In this work, incident light was assumed to be normally incident at a wavelength of 633 nm. The polarization state was  $x$ -linear polarization (XLP) propagating along the  $z$ -direction from bottom to up, as shown in Fig. 1a. The inclined angle between the  $x$ -axis and the long axis of the nano-fin was set at  $45^\circ$ . Under this assumption, the PCE and transmittance were identical to a circular polarized light normally incident on a nano-fin at an arbitrary rotation angle. The XLP incident light was denoted by  $E_{x-in}$ . After passing through the nano-fin, the polarization state varied because of the anisotropy of the nano-fin. Therefore, the output component of the  $E$ -field (denoted by  $E_{out}$ ) consisted of  $E_{x-out}$  and  $E_{y-out}$ , which represented  $E_x$  and  $E_y$  components at the output plane, respectively. The PCE can be calculated as follows:

$$\frac{|E_{y-out}|^2}{|E_{out}|^2} \times 100\% = \frac{|E_{y-out}|^2}{|E_{x-out}|^2 + |E_{y-out}|^2} \times 100\% \quad (1)$$

For PB-phase metasurfaces, the PCE is occasionally used to evaluate the efficiency. However, emphasis is mostly on the overall efficiency, which is the ratio of the signal light intensity to the incident light intensity. Therefore, transmittance and overall PCE must be determined.

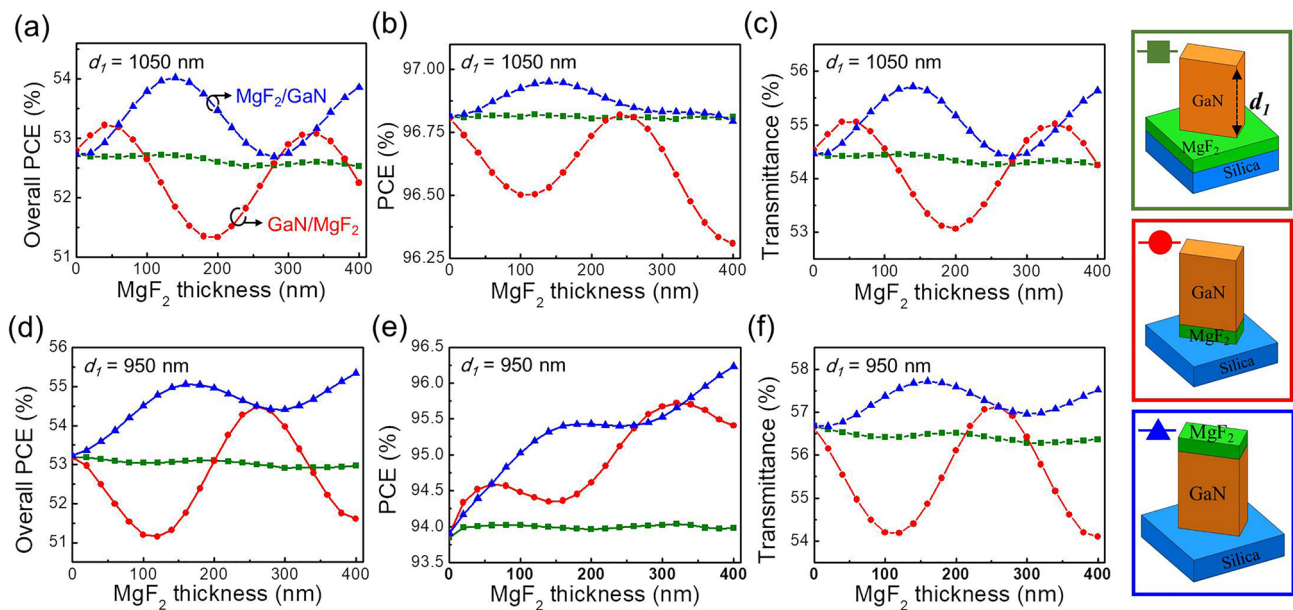
The transmittance is defined as follows:

$$\frac{|E_{out}|^2}{|E_{x-in}|^2} \times 100\% = \frac{|E_{x-out}|^2 + |E_{y-out}|^2}{|E_{x-in}|^2} \times 100\% \quad (2)$$

Finally, the overall PCE can be defined as PCE multiplied by transmittance, as given below:

$$\frac{|E_{y-out}|^2}{|E_{x-in}|^2} \times 100\% \quad (3)$$

The overall PCE is more appropriate for describing the overall efficiency of a PB-phase unit cell, which considers both transmittance and PCE. Figure 1b depicts the transmittance, PCE, and overall PCE as a function of the thickness ( $d_1$ ) of the GaN nano-fin. The square, circle, and triangle represent the transmittance, PCE, and



**Figure 2.** Optical property of GaN nano-fin consisted with  $\text{MgF}_2$  layer. Simulation results of (a) overall PCE, (b) PCE, and (c) transmittance versus  $\text{MgF}_2$  thickness with  $d_1 = 1050$  nm. Simulation results of (d) overall PCE, (e) PCE, and (f) transmittance of versus  $\text{MgF}_2$  thickness with  $d_1 = 950$  nm. The green square denotes a flat  $\text{MgF}_2$  film deposited under a GaN nano-fin, the red circle denotes a GaN nano-fin located on the top of the  $\text{MgF}_2$  nano-structure, and the blue triangle denotes a  $\text{MgF}_2$  nano-structure stacked on the top of a GaN nano-fin.

overall PCE, respectively. The peak of the PCE is at  $d_1 = 1050$  nm, corresponding to the half-waveplate condition for polarization conversion. However, due to the yellow-band absorption of GaN, caused by Ga vacancies or their complexes<sup>39,40</sup>, GaN is lossy at  $\lambda = 633$  nm and the corresponding refractive index is  $n + ik = 2.29 + 0.061i$ <sup>41</sup>. Therefore, transmittance decreased with an increase in thickness. After considering the contribution of transmittance, the highest overall PCE was believed to appear at  $d_1 = 950$  nm.

Here, we considered three different cases of the  $\text{MgF}_2$ -based antireflection structure for reducing the reflection loss of GaN nano-fins. The first was the GaN nano-fin deposited on a flat  $\text{MgF}_2$  film over a silica substrate, which is the most intuitive antireflection structure (denoted by the green square in Fig. 2). The second (denoted by the red circle) was a GaN nano-fin stacked on a  $\text{MgF}_2$  nano-fin, which was fabricated through standard lithography and reactive-ion etching. This is a hetero-nano-fin. For convenience, the second nano-fin is called the GaN/ $\text{MgF}_2$  nano-fin. Moreover, the  $\text{MgF}_2$  nano-structure had the same geometric parameters as the nano-fin in the x and y directions. Finally, the third nano-fin (denoted by the blue triangle) was a  $\text{MgF}_2$  nano-fin stacked on the GaN nano-fin and was called a  $\text{MgF}_2/\text{GaN}$  nano-fin. Same as the previous case, the geometric parameters of  $\text{MgF}_2$  and GaN nano-fins were identical in the x and y directions. The simulation results of the overall PCE, PCE, and transmittance as a function of  $\text{MgF}_2$  thickness are displayed in Fig. 2a–c, respectively. For  $d_1 = 1050$  nm, the flat  $\text{MgF}_2$  film (green square) barely contributed to the PCE, overall PCE, and transmittance even with an increase in the thickness. Therefore, this case was used as a reference. For the GaN/ $\text{MgF}_2$  nano-fin (red circle), a noticeable oscillation of overall PCE was observed with an increase in  $\text{MgF}_2$  thickness. When  $\text{MgF}_2$  thickness increased, the PCE curve oscillated and became lower, which was because the anisotropic OPD of nano-fin is away from the optimal optimized thickness of the half-waveplate (as mentioned in Fig. 1b). At the same time, the GaN/ $\text{MgF}_2$  nano-fin positively contributed to transmittance. Although a 0.5% increase in transmittance was observed for  $\text{MgF}_2 = 60$  nm, the transmittance was suppressed for most thicknesses. Notably, the overall PCE was significantly improved for the  $\text{MgF}_2/\text{GaN}$  nano-fin. The overall PCE increased from 52.7 to 54% when  $\text{MgF}_2$  thickness increased from 0 to 140 nm. Although the overall PCE oscillated with varying  $\text{MgF}_2$  thickness, the overall PCE constantly improved, compared with a bare GaN nano-fin. Because the GaN nano-fin with a thickness of 1050 nm already had the highest PCE, only a tiny increment was observed in the PCE after the addition of the  $\text{MgF}_2$  nano-structure. Therefore, improvement in the overall PCE is believed to be mainly contributed by transmittance. Figure 2c shows a good agreement that transmittance improves from 54.4 to 55.7%. Figure 2d–f depict the overall PCE, PCE, and transmittance for  $d_1 = 950$  nm, which is the optimal thickness of the bare GaN nano-fin for the overall PCE. Compared with  $d_1 = 1050$  nm, both GaN/ $\text{MgF}_2$  and  $\text{MgF}_2/\text{GaN}$  nano-fins showed an improved overall PCE for  $d_1 = 950$  nm, as shown in Fig. 2d. Both PCE and transmittance exhibited significant improvement. The  $\text{MgF}_2$  nano-structure simultaneously played a role in polarization conversion and antireflection. The increasing thickness allowed the anisotropic OPD to match the optimal half-waveplate condition. Therefore, the PCE for both GaN/ $\text{MgF}_2$  and  $\text{MgF}_2/\text{GaN}$  nano-fins improved with an increase in  $\text{MgF}_2$  thickness. For transmittance, behaviors of GaN/ $\text{MgF}_2$  and  $\text{MgF}_2/\text{GaN}$  differed with increasing  $\text{MgF}_2$  thickness. Although GaN/ $\text{MgF}_2$  enhanced transmittance to 1.3% at a  $\text{MgF}_2$  thickness of 260 nm, the transmittance was generally reduced for other thicknesses of  $\text{MgF}_2$ . By contrast, the transmittance of  $\text{MgF}_2/\text{GaN}$  was constantly improved

regardless of the variation in  $\text{MgF}_2$  thickness. The flat  $\text{MgF}_2$  layer made no contribution to overall PCE for both  $d_1 = 1050$  or  $950$  nm. This means that the hetero-structure is necessary for antireflection.

For a homogeneous medium, the Goos–Hanchen phase is  $\pi$  when the incident angle is less than the total reflection angle<sup>42</sup>. In our case, an optical anisotropic nano-fin was considered. The reflected phase is no more exactly equal to  $\pi$  owing to anisotropy, depolarization, and scattering. Here, a simple optical isolator was used for comparison. Right-circularly polarized (RCP) light normally impinges on an optical homogeneous and anisotropy film, that is, a half-waveplate. After traveling to the top of the film–air interface, part of the light reflects and back travels to the input plane. An antireflection structure allows incident and reflection beams to destructively interfere. The Jones matrix of the input and reflected light can be represented as follows:

$$E_{out} = R(-\theta) \begin{pmatrix} e^{-i\frac{\Gamma}{2}} & 0 \\ 0 & e^{i\frac{\Gamma}{2}} \end{pmatrix} R(\theta) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} R(-\theta) \begin{pmatrix} e^{-i\frac{\Gamma}{2}} & 0 \\ 0 & e^{i\frac{\Gamma}{2}} \end{pmatrix} R(\theta) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \quad (4)$$

where  $\theta$  is the phase retardation and  $R$  is the rotation matrix:

$$R(-\theta) = \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix} \quad (5)$$

As the RCP travels at the quarter-waveplate position, the polarization state converts to XLP. At the top of the film–air interface, polarization states of the incident and reflected light are left-circularly polarized (LCR) and RCP, respectively. When light back travels to the quarter-waveplate position, the polarization state converts to y-linear polarization. Finally, at the input plane, the back-reflected light is LCP, which is orthogonal to the input light. Thus, the vector product of the input and reflected light is zero. Therefore, the input and reflected light cannot interfere, and thus, a conventional thin-film antireflection coating is not suitable for reducing the Fresnel reflection loss of a homogeneous and anisotropy film.

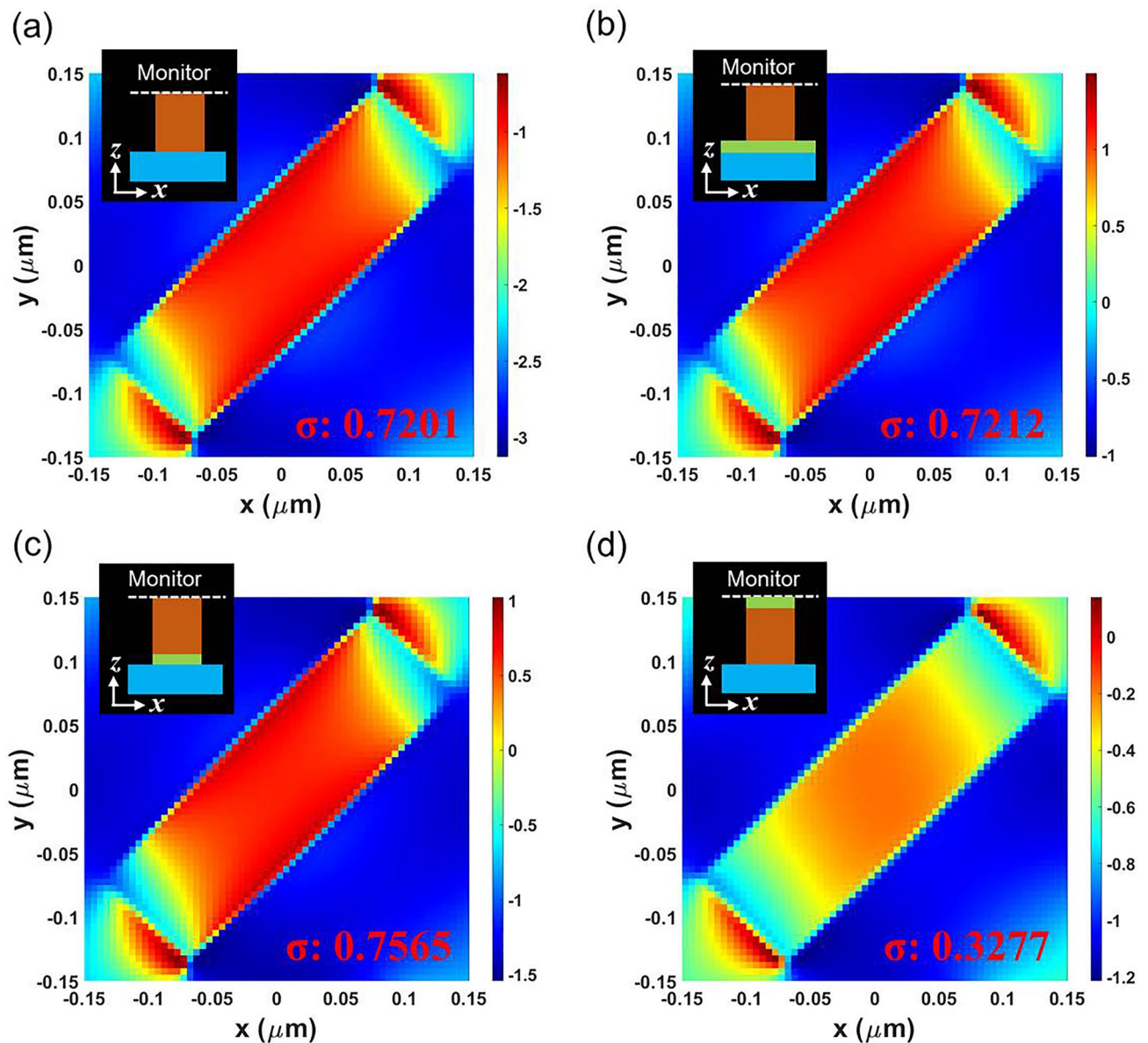
In our nano-fin, the Goos–Hanchen reflection phase from the structure is not only equal to  $\pi$  but also has phase anisotropy. Therefore, polarization states of forward and backward propagation light are not completely orthogonal in our discussed PB-phase nano-fin system. We thus can realize antireflection in the PB-phase system.

Figure 3 presents the phase distribution at the upper interface of the nano-fin coated with four antireflection structures: bare nano-fin, nano-fin with a flat  $\text{MgF}_2$  film,  $\text{GaN}/\text{MgF}_2$  nano-fin, and  $\text{MgF}_2/\text{GaN}$  nano-fin. The corresponding phase distributions are presented in Fig. 3a–d. Here, the thickness of  $\text{GaN}$  and  $\text{MgF}_2$  was fixed at 950 and 140 nm, respectively. To analyze phase distribution intuitively, we calculated the standard deviation of the phase and marked it as  $\sigma$ . Figure 3a depicts that the  $\sigma$  of the bare nano-fin is 0.7201, which can be considered as a reference. We first observed that the  $\sigma$  of the nano-fin with the flat  $\text{MgF}_2$  film was 0.7212, as shown in Fig. 3b. Compared with the reference, the flat  $\text{MgF}_2$  film contributed inconspicuously to the antireflection effect. The  $\sigma$  of the  $\text{GaN}/\text{MgF}_2$  nano-fin was 0.7565. Compared with the flat  $\text{MgF}_2$  film, phase distribution on the interface changed drastically, corresponding to the decreases in efficiency. As shown in Fig. 2d, the  $\text{GaN}/\text{MgF}_2$  nano-fin exhibited lower overall PCE at a  $\text{MgF}_2$  thickness of 140 nm. Finally, the  $\sigma$  of the  $\text{MgF}_2/\text{GaN}$  nano-fin was 0.3277, as shown in Fig. 3d. Compared with the flat  $\text{MgF}_2$  film, the variation in phase distribution on the interface was mitigated and transmittance was increased.

As mentioned above,  $\text{GaN}$  suffers from absorption loss in the visible range. The optical characteristics of material loss make improving the overall PCE difficult. Therefore, materials without absorption loss in the visible range must be identified. For example, Choudhury et al. comprehensively surveyed a dielectric material for a dielectric metasurface for visible and IR spectral ranges<sup>43</sup>. They suggested silicon nitride ( $\text{Si}_3\text{N}_4$ ) and titanium oxide ( $\text{TiO}_2$ ) as good metasurfaces in visible range applications.

In addition to absorption loss, the refractive index is crucial for fabrication. Both the propagation phase and anisotropy are positively related to the refractive index. Therefore, a high aspect ratio is required to accumulate sufficient phase modulation for materials with a relatively low refractive index. We thus focused on dielectric materials that can be applied in the visible range and have a high refractive index. Figure 4 depicts the optimized thickness ( $d_2$ ) of nano-fins based on various materials. As shown in the inset of Fig. 4, geometric parameters were all fixed (length, 300 nm; width, 100 nm; and period, 330 nm). Recently, Prof. Tsai's group demonstrated a  $\text{GaN}$  structure with an aspect ratio as high as 10–20 for high efficiency<sup>18,44,45</sup>. However, fabricating a nano-fin with such a high aspect ratio is extremely challenging. Thus, we used the geometric parameters of the  $\text{GaN}$  nano-fin as a benchmark for the state-of-the-art fabrication. Nano-fins with an optimized thickness higher than that of  $\text{GaN}$  nano-fin were excluded as candidates for a high-efficiency dielectric metasurface. According to this criterion,  $\text{Si}_3\text{N}_4$ , tantalum pentoxide ( $\text{Ta}_2\text{O}_5$ ), and sputtering  $\text{TiO}_2$  are not suitable materials. Compared with  $\text{GaN}$ , both anatase and rutile  $\text{TiO}_2$  have the advantages of higher efficiency and lower aspect ratio. However, the crystalline phase control of  $\text{TiO}_2$  during deposition is severe. Thus, crystalline  $\text{TiO}_2$  is also excluded. Amorphous silicon (a-Si) is a material with a high refractive index and can be easily processed using standard semiconductor-compatible manufacturing techniques. However, it suffers from huge absorption loss in the visible range, which makes it inappropriate. Finally,  $\text{Nb}_2\text{O}_5$  offers a fair refractive index and low absorption ( $n + ik = 2.32 + 0i$ ), making it suitable for visible applications. Therefore, we believe that  $\text{Nb}_2\text{O}_5$  is suitable for high-efficient dielectric metasurfaces.

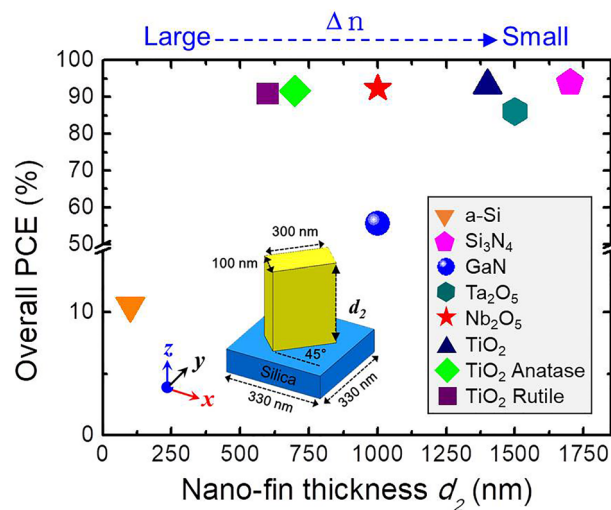
We simulated the optical response of a nano-fin composed of  $\text{Nb}_2\text{O}_5$  patterned on the same substrate at an incident wavelength of 633 nm, as shown in Fig. 5a. The polarization state was XLP propagating along the z-direction. Figure 5b depicts the transmittance, PCE, and overall PCE as a function of the thickness ( $d_3$ ) of the  $\text{Nb}_2\text{O}_5$  nano-fin. Corresponding to the half-waveplate condition for polarization conversion, the peak of the PCE appeared at  $d_3 = 1000$  nm. Because  $\text{Nb}_2\text{O}_5$  does not suffer absorption loss in the visible range, which can be easily observed, transmittance did not decrease with an increase in  $d_3$ . Therefore, same as the PCE, the highest



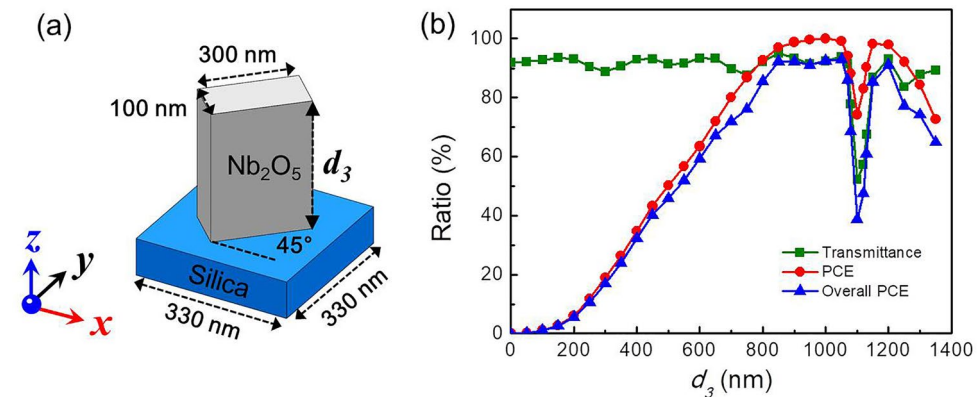
**Figure 3.** Electric field distribution of nano-fin structures. Simulations of phase distribution at the upper interface of the nano-fin for the (a) nano-fin without  $\text{MgF}_2$ , (b) flat  $\text{MgF}_2$  film, (c) nano-fin stacking on the  $\text{MgF}_2$  nano-structure, and (d)  $\text{MgF}_2$  nano-structure stacking on a nano-fin.  $\sigma$  is the standard deviation of phase distribution at the upper interface.

overall PCE appeared at  $d_3 = 1000$  nm. As expected, the overall PCE of  $\text{Nb}_2\text{O}_5$  was considerably higher than that of the GaN nano-fin. By contrast, an obvious dip appeared at  $d_3 = 1100$  nm, which is caused by guided-mode resonance<sup>46</sup>.

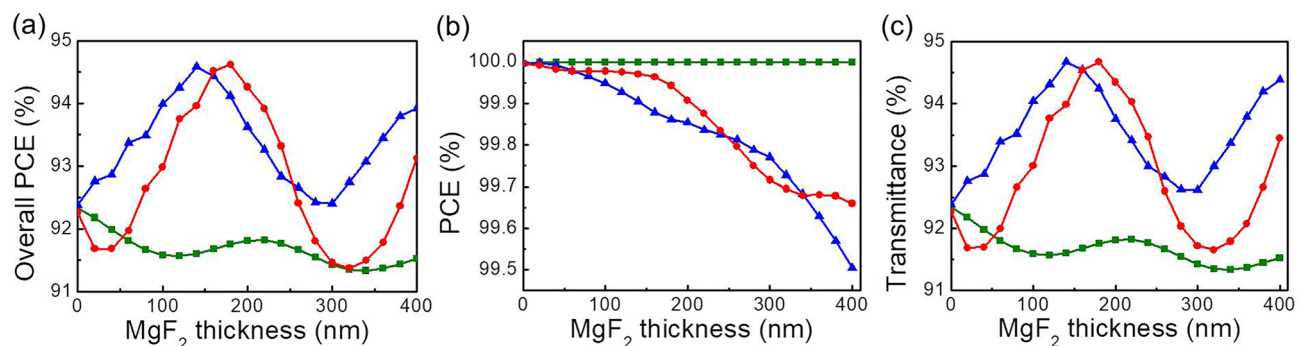
We also considered three different cases of the  $\text{MgF}_2$ -based antireflection layer for reducing the reflection loss of the  $\text{Nb}_2\text{O}_5$  nano-fin: a flat  $\text{MgF}_2$  film under the nano-fin,  $\text{Nb}_2\text{O}_5/\text{MgF}_2$  nano-fin, and  $\text{MgF}_2/\text{Nb}_2\text{O}_5$  nano-fin, which are denoted by a green square, red circle, and blue triangle, respectively, in Fig. 6. Here, the thickness ( $d_3$ ) of  $\text{Nb}_2\text{O}_5$  for all cases was 1000 nm. The simulation results of the overall PCE, PCE, and transmittance as a function of  $\text{MgF}_2$  thickness are presented in Fig. 6a–c, respectively. First, a flat  $\text{MgF}_2$  film in the  $\text{Nb}_2\text{O}_5$  system barely contributed to the PCE, overall PCE, and transmittance. Therefore, this case was marked as a reference. Both  $\text{Nb}_2\text{O}_5/\text{MgF}_2$  and  $\text{MgF}_2/\text{Nb}_2\text{O}_5$  nano-fins exhibited obvious enhancement of the overall PCE (Fig. 6a). The highest overall PCE of both  $\text{Nb}_2\text{O}_5/\text{MgF}_2$  and  $\text{MgF}_2/\text{Nb}_2\text{O}_5$  nano-fins was 94.6% when  $\text{MgF}_2$  thickness was 160 and 140 nm, respectively. The thickness of the  $\text{Nb}_2\text{O}_5$  nano-fin ( $d_3 = 1000$  nm) was already an optimal optimized half-waveplate. For both  $\text{Nb}_2\text{O}_5/\text{MgF}_2$  and  $\text{MgF}_2/\text{Nb}_2\text{O}_5$  nano-fins, an additional  $\text{MgF}_2$  layer forced the nano-fin away from the optimal optimized thickness of the half-waveplate and decreased the PCE (Fig. 6b). Thus, transmittance enhancement contributed to all the improvement in the overall PCE. Figure 6c shows a transmittance of 94.7% for both  $\text{Nb}_2\text{O}_5/\text{MgF}_2$  and  $\text{MgF}_2/\text{Nb}_2\text{O}_5$  nano-fins. Although both these nano-fins exhibited a good



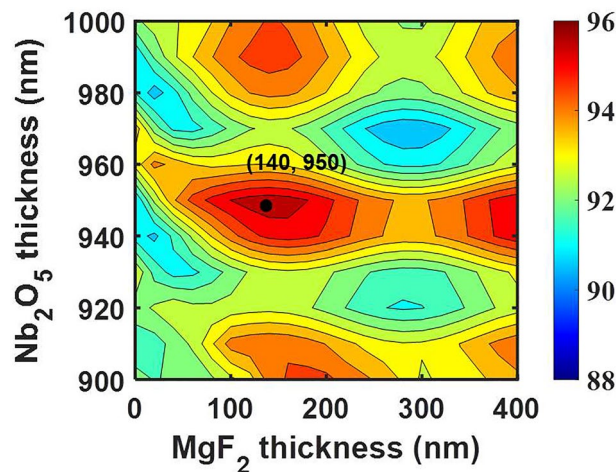
**Figure 4.** Overall PCE comparison. Optimized thickness ( $d_2$ ) of a nano-fin for various materials at the highest overall PCE. The geometric diagram of a meta-atom is shown in inset.



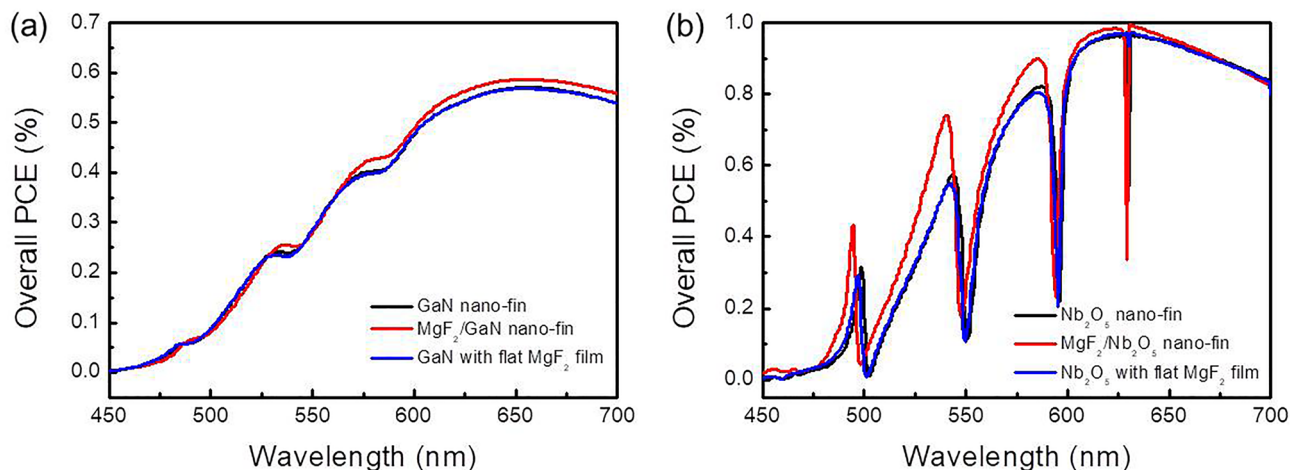
**Figure 5.** Geometric diagram and optical property of  $\text{Nb}_2\text{O}_5$  nano-fin. (a) Schematic of a  $\text{Nb}_2\text{O}_5$  nano-fin on a silica substrate, where  $d_3$  is the thickness of the  $\text{Nb}_2\text{O}_5$  nano-fin. (b) Transmittance, PCE, and overall PCE versus the thickness of the  $\text{Nb}_2\text{O}_5$  nano-fin. x-polarized light with  $\lambda = 633$  nm impinges perpendicularly onto the structure from bottom along the positive z-direction.



**Figure 6.** Optical property of  $\text{Nb}_2\text{O}_5$  nano-fin consisted with  $\text{MgF}_2$ . Simulation results of (a) overall PCE, (b) PCE, and (c) transmittance as a function of  $\text{MgF}_2$  thickness. The thickness of  $\text{Nb}_2\text{O}_5$  is fixed to be  $d_3 = 1000$  nm. The green square denotes a flat  $\text{MgF}_2$  film deposited under the  $\text{Nb}_2\text{O}_5$  nano-fin, the red circle denotes a nano-fin located on the top of the  $\text{MgF}_2$  nano-structure, and the blue triangle denotes a  $\text{MgF}_2$  nano-structure stacked on the top of a nano-fin.



**Figure 7.** Overall PCE mapping of  $\text{MgF}_2/\text{Nb}_2\text{O}_5$  hetero-nano-fin. Simulation of overall PCE as a function of  $\text{MgF}_2$  and  $\text{Nb}_2\text{O}_5$  thicknesses.  $\text{MgF}_2$  is located on the top of the  $\text{Nb}_2\text{O}_5$  nano-fin. The black dot represents the thickness with the highest overall PCE.



**Figure 8.** Simulation results of overall PCE spectra. (a) GaN nano-fin and flat  $\text{MgF}_2$  film thickness are 950 nm and 140 nm, respectively. In the hetero-nano-fin case, GaN and  $\text{MgF}_2$  thickness is 950 nm and 140 nm. (b) For the case of flat  $\text{MgF}_2$  film, the thickness of  $\text{Nb}_2\text{O}_5$  nano-fin and flat  $\text{MgF}_2$  film is 1000 nm and 140 nm, respectively. In the hetero-nano-fin case,  $\text{Nb}_2\text{O}_5$  nano-fin and flat  $\text{MgF}_2$  film thickness is 950 nm and 140 nm, corresponding to the highest overall PCE condition.

enhancement of the overall PCE, the  $\text{MgF}_2/\text{Nb}_2\text{O}_5$  nano-fin attained thickness efficiency at a lower  $\text{MgF}_2$  thickness. Thus, the antireflection layer located on the top of a nano-fin is considered more suitable.

As mentioned above,  $\text{MgF}_2$  contributed negatively to the PCE and reduced the overall PCE when the nano-fin thickness was under an ideal half-waveplate condition. Therefore, we further optimized the hetero-nano-fin to ensure that the  $\text{Nb}_2\text{O}_5$  nano-fin was slightly thinner than the ideal half-waveplate condition. Figure 7 presents the overall PCE as a function of  $\text{MgF}_2$  and  $\text{Nb}_2\text{O}_5$  thicknesses. The color represents the overall PCE. Warm and cold colors represent the enhanced and suppressed overall PCE, respectively, compared with the bare  $\text{Nb}_2\text{O}_5$  nano-fin. In this calculation,  $\text{MgF}_2$  was located on the top of the  $\text{Nb}_2\text{O}_5$  nano-fin. As the thickness of  $\text{Nb}_2\text{O}_5$  was 950 nm, the overall PCE improved from 91 to 96% when  $\text{MgF}_2$  thickness increased from 0 to 140 nm. At this time,  $\text{MgF}_2$  made up for a shortage in the ideal half-waveplate condition.  $\text{MgF}_2$  plays a role in both polarization conversion and antireflection. Moreover, the overall PCE of the  $\text{MgF}_2/\text{Nb}_2\text{O}_5$  nano-fin was 1.7 times higher than that of the  $\text{MgF}_2/\text{GaN}$  nano-fin. Therefore, we believe that the  $\text{MgF}_2/\text{Nb}_2\text{O}_5$  hetero-nano-fin is a highly efficient candidate for dielectric metasurfaces.

We further investigated the overall PCE enhancement of hetero-nano-fin in the visible wave band. Figure 8a depicts the overall PCE of  $\text{MgF}_2/\text{GaN}$  hetero-nano-fin under normal illumination from 450 to 700 nm. Here, the thickness of GaN and  $\text{MgF}_2$  is 950 nm and 140 nm, corresponding to the highest overall PCE condition. We observed that the antireflection nano-fin worked from 530 to 545 nm and 560 nm to 700 nm. However, the

hetero-nano-fin was optimized for 633 nm application. Therefore, the overall PCE enhancement of  $\text{MgF}_2/\text{GaN}$  nano-fin in the red band is more evident than the blue and green bands. We next investigated the overall PCE enhancement of  $\text{MgF}_2/\text{Nb}_2\text{O}_5$  hetero-nano-fin. Here, the thickness of  $\text{MgF}_2$  and  $\text{Nb}_2\text{O}_5$  is 140 nm and 950 nm, respectively. In the case of flat  $\text{MgF}_2$  (marked as reference), the thickness of  $\text{MgF}_2$  and  $\text{Nb}_2\text{O}_5$  is 140 nm and 1000 nm, corresponding to the highest overall PCE condition. Figure 8b presents that the additional antireflection structure significantly improves efficiency. Compared with the reference, hetero-nano-fin's average overall PCE enhancement is 4.3% from 450 to 700 nm. By contrast, four noticeable dips appear which were caused by guided-mode resonance.

## Conclusions

In summary, we numerically investigated the enhancement of overall PCE of hetero-nano-fins by using GaN and  $\text{Nb}_2\text{O}_5$  nano-fins with three types of antireflection structure: an intuitive flat  $\text{MgF}_2$  layer under nano-fins, nano-fins/ $\text{MgF}_2$ , and  $\text{MgF}_2$ /nano-fins. Compared with the flat antireflection layer, a hetero-nano-fin exhibited a better overall PCE enhancement. Both GaN/ $\text{MgF}_2$  and  $\text{MgF}_2$ /GaN nano-fins improved PCE with an increase in  $\text{MgF}_2$  thickness. Compared with the GaN/ $\text{MgF}_2$  nano-fin, the  $\text{MgF}_2$ /GaN nano-fin led to higher overall PCE enhancement. For the  $\text{MgF}_2$ /GaN nano-fin, the overall PCE improved from 52.7% to 54% with an increase in  $\text{MgF}_2$  thickness from 0 to 140 nm. Unfortunately, the absorption loss of GaN in the visible range limited its overall PCE. By contrast, lossless  $\text{Nb}_2\text{O}_5$  was considered because of its high refractive index. The overall PCE of the  $\text{Nb}_2\text{O}_5$ -based nano-fin was 1.7 times higher than that of the GaN-based nano-fin. Moreover, an overall PCE up to 96% was achieved after optimization. The overall PCE spectra show that  $\text{Nb}_2\text{O}_5$ -based hetero-nano-fin's average overall PCE enhancement is 4.3% from 450 to 700 nm. Antireflection coating for a metasurface is crucial for enhancing the efficiency and reducing the background signal of a meta-device.

## Methods

All simulation results were performed with the FDTD methods. All nano-fins were simulated with periodic boundary conditions in xz and yz-planes; absorbing boundary in xy-planes. The incident wavelength was 633 nm with x-polarized. The refractive index of silica substrate, GaN, and  $\text{Nb}_2\text{O}_5$  are  $1.45 + 0i$ ,  $2.29 + 0.061i$ , and  $2.32 + 0i$  at 633 nm, respectively. The refractive index of  $\text{Nb}_2\text{O}_5$  is measured by spectroscopic ellipsometry. The 3D model of an infinite array of dielectric nano-fins implemented periodic boundary conditions (PBC) on the sides and perfectly matched layers (PML) on the top and the bottom of the simulation domain. The mesh size was set to be smaller than 5 nm. The nano-fins were excited by a normal-incidence plane wave from the substrate-side.

## Data availability

All data generated or analysed during this study are included in this published article (and its Supplementary Information files).

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## Author contributions

Y.-H. L. and W.-L. H. designed and performed the simulations and data analysis; C.-Y. Y. performed the simulations. W.-L. H. wrote the manuscript; C.-M. W. developed the theoretical aspect, analyzed the result, and prepared the manuscript. All authors commented on the manuscript.

## Competing interests

The authors declare no competing interests.

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