

## 基于光学薄膜的高效超构表面研究

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**摘要** 超构表面(metasurfaces)是一种新型的人工二维平面阵列结构,通过合理设计亚波长纳米结构单元及排布可以实现对空间光场的调控,有望从原理层面上颠覆传统的透镜元件。然而,目前透射型超构表面普遍存在光学效率低的问题,制约着其应用和发展。首次提出了光学薄膜结合超构表面提高光能利用率的设想,期望超构表面结合光学薄膜的结构在不影响超构表面光学特性的基础上,可以显著地提高其光学效率。为了验证这一策略的有效性,仿真模拟了石英基底近红外宽波段的硅纳米块超构表面透镜,并与设计有光学薄膜的超构表面进行了对比。模拟结果表明:光学薄膜对超构表面的聚焦性能没有影响,但可以显著提高超构表面的光学透过率;在1450~1600 nm波段,平均透过率提高了10.5%以上,聚焦效率平均提高了8.3%以上。所提方法为超构表面器件设计带来了新的思路。

**关键词** 超构表面; 光学薄膜; 硅纳米块; 透过率

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## 1 引言

近年来,超构表面作为光学领域中一种极富创新性的概念吸引了人们广泛的关注<sup>[1-2]</sup>。超构表面是由许多亚波长纳米结构单元组成的二维功能性平面结构,通过利用亚波长结构与入射光场的相互作用可以实现对空间光场的强度、相位及偏振等的高效调控,有望从原理层面上颠覆传统的光学元件和功能<sup>[3-5]</sup>。由超构表面制成的超构透镜轻薄扁平,能够实现对光波的有效聚焦和成像<sup>[6-9]</sup>,将可能取代传统光学系统中复杂笨重的透镜组,使得手机、相机、监控摄像头等产品都变得小巧轻薄,因而成为了光学领域的一项革命性技术并引领了一场研究的热潮。

目前,在超构表面结构设计方面,主要分为金属天线阵列超构表面<sup>[10]</sup>、全介质超构表面<sup>[11]</sup>和金属-介质混合超构表面<sup>[12]</sup>设计。然而,无论是哪种设计结构,都存在着聚焦效率低的问题。具体来说,金属超构表面和金属-介质混合超构表面由于电磁波与金属自由电子的相互作用会产生很强的损耗,因而基于金属孔或金属纳米天线构造的超构表面阵列所设计的透镜的透过率及光能利用率不高<sup>[13-14]</sup>。基于全介质纳米单元结构设计的超构表面虽然比金属超构表面在效率上有很大的提升,但单元结构散射损失依然比较大<sup>[15]</sup>。此外,为了降低超构表面的厚度和制备工艺难度,介质超构表面一般由与光波波长可比拟长度的高折射率介质柱构成,但高折射率超构表面等效折射率较大,这样超构表

面层的等效导纳与入射介质、基底不匹配及超构表面高度与设计波长不匹配会导致极大的界面反射损失。在提高超构表面器件效率问题上,目前的研究主要集中在提高超构表面衍射效率,减少散射损失上。但对于超构表面的反射损失现在还鲜有研究。

针对上述透射型超构表面存在界面反射损失的问题,提出了一种基于光学薄膜理论的高效透射型超构表面设计方案。先设计好超构表面,然后根据等效介质理论将超构表面等效为一层介质薄膜并作为多层膜系的最外层,最后设计与基底及入射介质匹配的增透膜系。希望增加的光学膜层能提高光能利用率,但不改变超构表面的其他光学性质。换句话说,超构表面在实现聚焦或其他功能的同时,还能像传统透镜表面一样兼容功能性光学薄膜,从而在性能上获得进一步的提高和拓展。

## 2 理论模型

透镜作为光学系统中最重要和最基本的元件,在光学系统中发挥着至关重要的作用。为了验证基于光学薄膜理论的高效超构表面设计方案的正确性,设计了具有增透膜系的透射型超构表面透镜,并对其光学性质进行了具体的仿真模拟。基底为石英材料,超构表面介质柱为Si材料,采用FDTD(finite-difference time-domain)法模拟计算了基于这两种材料做成的超构表面透镜的光学性质。

超构表面透镜单元结构如图1所示,分为三部分,

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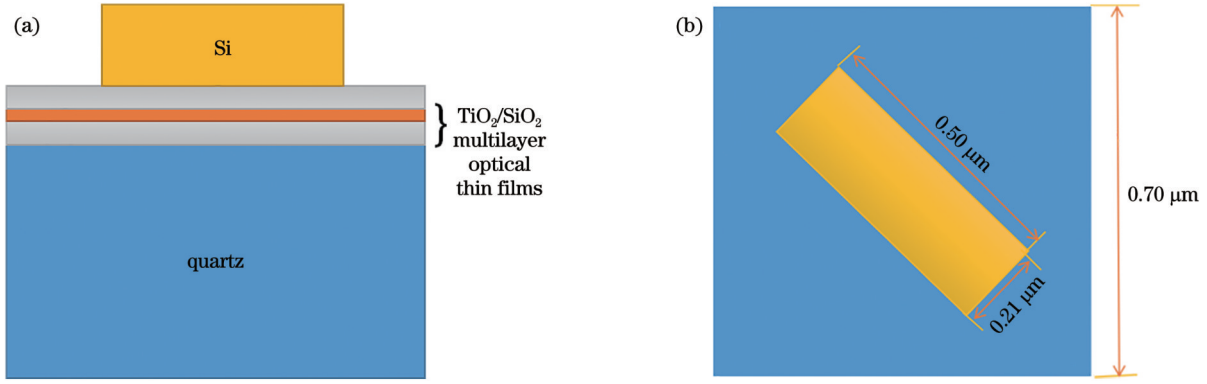


图 1 设计有光学薄膜的超构表面结构示意图。(a)单元结构截面示意图;(b)单元结构俯视图

Fig. 1 Schematic diagrams of the metasurface structure with optical thin film. (a) Section diagram of unit structure; (b) top view diagram of unit structure

最上面为超构表面层,中间部分为多层光学薄膜,最下面是石英基底。超构表面单个纳米块结构为长  $0.50 \mu\text{m}$ 、宽  $0.21 \mu\text{m}$ 、高  $0.50 \mu\text{m}$  并沿固定的方向取向的长方体。这些纳米块单元空间规律性排布组成了超构表面,其周期为  $0.7 \mu\text{m} \times 0.7 \mu\text{m}$ ,入射光束为直径  $30 \mu\text{m}$  的左旋圆偏振平面光。

图 2 是在波长为  $1.53 \mu\text{m}$  的偏振光入射时,随着纳米块方位角改变对应的相位延迟,可以看出,纳米块方位角在  $0 \sim \pi$  范围内变化,相位延迟覆盖  $0 \sim 2\pi$  范围。超构表面透镜采用双曲面形的相位场(消纵向球差双曲相位)分布来构建一个球面波前,整个超构表面透镜直径为  $30 \mu\text{m}$ ,具有相同方位角的单元结构组成一个

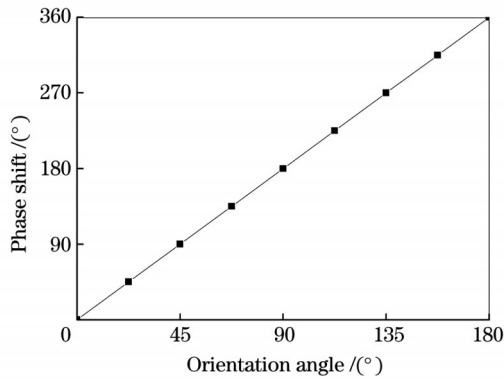


图 2 1530 nm 波长处硅纳米块不同方位角对应的相位变化  
Fig. 2 Phase change as a function of azimuthal angle of silicon nanobricks at the wavelength of 1530 nm

同心圆环。对于波长为  $\lambda$  的正入射光束,其相位场分布<sup>[16]</sup>为

$$\varphi(x, y) = \frac{2\pi}{\lambda} \left( f - \sqrt{x^2 + y^2 + f^2} \right), \quad (1)$$

式中: $f$ 为透镜的焦距; $(x, y)$ 为纳米单元结构的位置坐标。

如前所述,为了验证光学薄膜对超构表面器件性能的影响,将超构表面等效为一层光学薄膜并设计了针对基底的增透膜,超构表面的等效折射率使用等效介质理论计算。等效介质理论是比较直观的研究亚波长结构的近似理论<sup>[17]</sup>,当入射波长大于超构表面特征尺寸时,不会激发光波的高阶衍射,因此将超构表面等效为一层均匀介质薄膜是合理的。所设计的超构表面特征尺寸远小于光波长,所以可以使用等效介质理论计算。通过介质等效后,可采用光学薄膜理论设计增透膜系。等效薄膜折射率近似计算公式<sup>[18]</sup>表示为

$$n_{\text{eff}} = \left[ d_c n_{\text{si}}^q + (1 - d_c) n_{\text{air}}^q \right]^{\frac{1}{q}}, \quad (2)$$

式中: $d_c$ 为纳米块占空比; $n_{\text{si}}$ 为硅折射率,取值 3.6; $n_{\text{air}}$ 为空气折射率,取值 1; $q$ 为常数 2。增透膜材料选择在近红外透明且与基底及超构表面结合牢固的  $\text{TiO}_2$  和  $\text{SiO}_2$  材料。采用多层膜传输矩阵理论对膜系进行计算<sup>[19]</sup>,不考虑膜系的吸收和散射损耗的情况下,入射电磁场( $E_i$ 和 $H_i$ )和出射电磁场( $E_t$ 和 $H_t$ )之间的关系<sup>[20]</sup>表示为

$$\begin{bmatrix} E_t \\ H_t \end{bmatrix} = \begin{bmatrix} B \\ C \end{bmatrix} \begin{bmatrix} E_i \\ H_i \end{bmatrix} = \left\{ \prod_{i=1}^N \begin{bmatrix} \cos \delta_i & \frac{i}{\eta_i} \sin \delta_i \\ i\eta_i \sin \delta_i & \cos \delta_i \end{bmatrix} \right\} \begin{bmatrix} 1 \\ \eta_{N+1} \end{bmatrix} \begin{bmatrix} E_i \\ H_i \end{bmatrix}, \quad (3)$$

式中: $\delta_i = \frac{2\pi}{\lambda} n_i d_i$ (其中, $n_i$ 为第  $i$  层薄膜的折射率, $d_i$ 为第  $i$  层薄膜的物理厚度)为第  $i$  层薄膜的相位厚度; $\eta_i$ 为第  $i$  层材料导纳; $\eta_{N+1}$ 为基底导纳。在计算中,令有

等效导纳  $Y = \frac{C}{B} = n_0$ ( $n_0$ 为空气折射率)。图 3 为采用等效介质理论计算得到的硅纳米块阵列超构表面等效折射率。在  $1400 \sim 1650 \text{ nm}$  波段,消光系数为 0,折射率

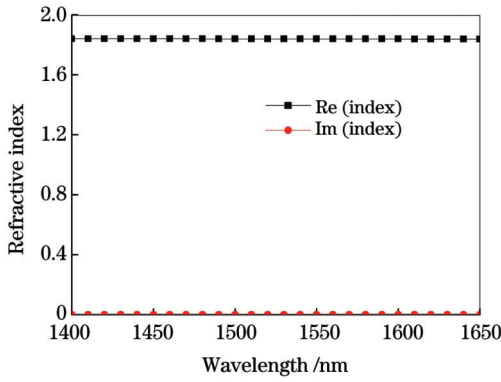


图 3 超构表面等效折射率

Fig. 3 Equivalent refractive index of metasurfaces

色散非常小(可以忽略不计),折射率约为 1.84。

### 3 结果与分析

当中心波长  $\lambda_0$  为 1530 nm 时,所设计的增透膜系为 Sub/0.2580H/1.1190L/2.1390H/2.9680L/0.9897H/2.3525L/MS/Air, 其中:H 表示光学厚度为  $\lambda_0/4$  的  $\text{TiO}_2$  膜层;L 表示光学厚度为  $\lambda_0/4$  的  $\text{SiO}_2$  膜层;H 和 L 前面的系数表示  $\lambda_0/4$  光学厚度的倍数,由膜层光学厚度换算成以  $\lambda_0/4$  为单位得到;MS 表示超构表面等效膜层,厚度为超构表面高度。采用固定膜层材料,把膜层厚度作为设计参数,最后计算得到膜系结构。图 4 为所设计的光学增透膜系与单层超构表面等效薄膜的透过率对比。从图 4 可以明显看出,增透膜系的透过率远大于超构表面等效膜层的透过率,平均透过率高出 12.4%。超构表面等效薄膜的透过率低主要是等效折射率和基底不匹配及等效薄膜的光学厚度与光波长不匹配产生反射的缘故。根据光学薄膜理论,光垂直入射超构表面等效薄膜时的反射率<sup>[21]</sup>为

$$R = \frac{(n_0 - n_2)^2 \cos^2 \delta_1 + (n_0 n_2 / n_1 - n_1)^2 \sin^2 \delta_1}{(n_0 + n_2)^2 \cos^2 \delta_1 + (n_0 n_2 / n_1 + n_1)^2 \sin^2 \delta_1}, \quad (4)$$

式中: $\delta_1 = \frac{2\pi}{\lambda} n_1 d_1$  为超构表面等效薄膜相位厚度; $n_1$

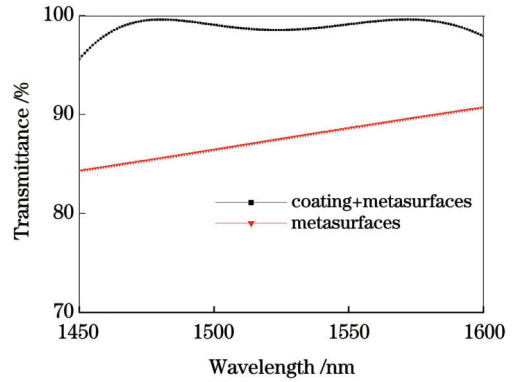


图 4 光学增透膜系与单层超构表面等效薄膜透过率对比

Fig. 4 Comparison of transmittance between optical antireflection coating system and single-layer metasurface equivalent thin film

为超构表面等效薄膜折射率; $d_1$  为超构表面厚度; $n_2$  为基底折射率。从式(4)可以看出,只有满足超构表面等效薄膜相位厚度  $\delta_1$  为  $\pi/2$  的整数倍及  $n_1 = \sqrt{n_0 n_2}$  时,在参考波长处的反射率才能达到最小值 0。通常超构表面不能满足上述条件,所以需要结合光学薄膜来减小光能反射损失。

图 5~7 对比了超构表面透镜在没有附加光学薄膜和附加光学薄膜(光学薄膜结合超构表面的增透膜系结构)时在不同波长(1460、1530、1600 nm)下的光场分布图。从图 5~7 可以看出:相同波长的两种结构超构表面的聚焦焦斑大小及焦距基本相同。有光学薄膜的情况下,焦点处光强度明显大于无光学薄膜时的强度,但焦点位置不受增透膜影响,基本没有变化。这说明光学薄膜只增加超构表面的透过率,对于其聚焦性能基本不产生影响。此外,从图 5~7 还可以看出,随着波长增加,焦距减小,这是因为超构表面对波长大的光衍射能力更强的缘故。不同波长(1460、1530、1600 nm)处无光学薄膜时的半峰全宽(FWHM)依次为 1.21、1.38、1.29  $\mu\text{m}$ ;有光学薄膜时 FWHM 依次为 1.23、1.41、1.28  $\mu\text{m}$ 。可以看出,相同波长下 FWHM

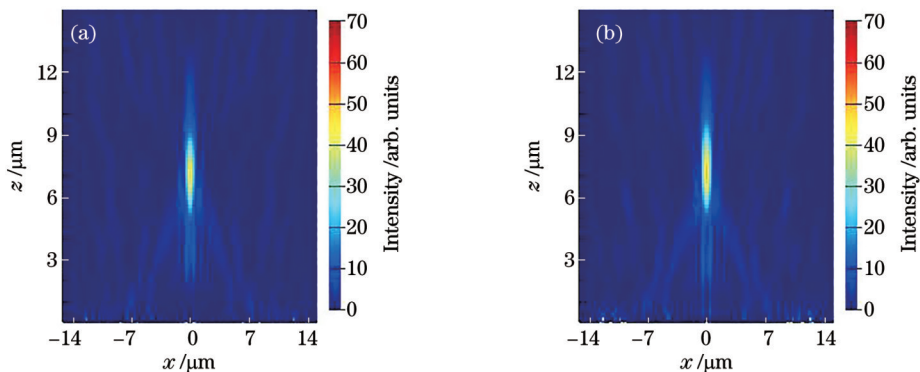


图 5 波长 1460 nm 处超构表面透镜的光场分布。(a) 无附加光学薄膜;(b) 附加光学薄膜

Fig. 5 Light field distributions of metasurface lens at a wavelength of 1460 nm. (a) Without optical thin films; (b) attached with optical thin films

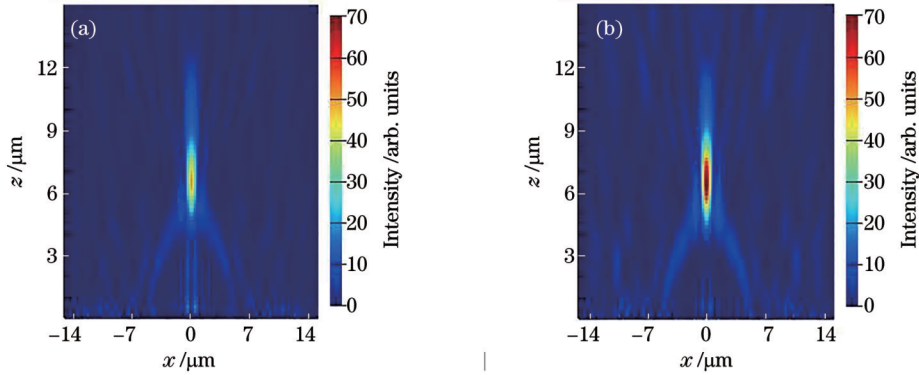


图 6 波长 1530 nm 处超构表面透镜的光场分布。(a) 无附加光学薄膜；(b) 附加光学薄膜

Fig. 6 Light field distributions of metasurface lens at a wavelength of 1530 nm. (a) Without optical thin films; (b) attached with optical thin films

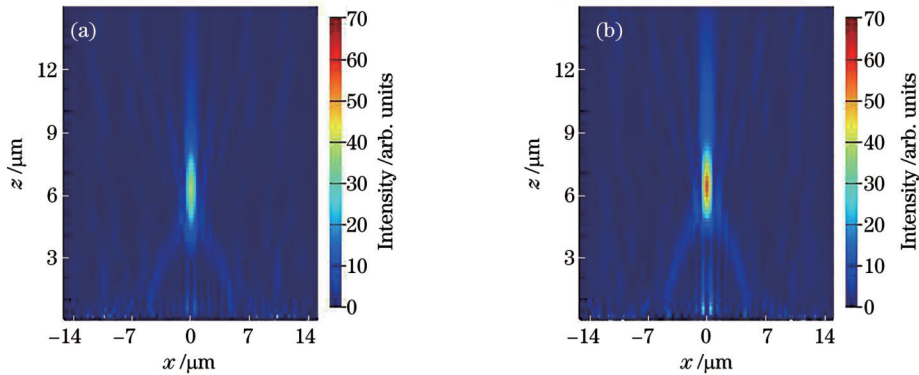


图 7 波长 1600 nm 处超构表面透镜的光场分布。(a) 无附加光学薄膜；(b) 附加光学薄膜

Fig. 7 Light field distributions of metasurface lens at a wavelength of 1600 nm. (a) Without optical thin films; (b) attached with optical thin films

基本一样,说明光学薄膜也不影响FWHM的大小。超构表面层增加多层光学薄膜并不改变超构表面透镜的焦距及超构表面的性能,却可以提高超构表面的效率。这是因为光学薄膜在整个面不会引入相位梯度变化,也就不会改变超构表面的功能,只是提高了光的透过率,超构表面的功能还是由纳米结构单元引入的相位梯度变化来实现。由于超构表面特征尺寸小于作用波长,对于传输相位和几何相位等类型超构表面,当光波入射超构表面时,类似于通过一等效的均匀薄膜,所以这种类型的超构表面都可以利用超构表面结合光学薄膜的方法来提高其光学效率。但是该方法不适合反射型超构表面,因为光学薄膜层会影响底层金属层与金属纳米结构局域等离子体谐振,进而影响反射相位。模拟计算的结果表明,所提光学薄膜与超构表面结合的设想是合理的,有望被应用于实际的超构表面制作中。

图 8 和图 9 为模拟计算得到的 1450~1600 nm 波段的透过率曲线及在 1450、1490、1530、1565、1600 nm 波长处的聚焦效率。从透过率曲线可以看出,在 1450~1600 nm 波段,设计有光学薄膜的超构表面透镜的透过率保持在 94.0% 左右,最高峰值达到 95.5%,远高于无光学薄膜时的透过率(平均高 10.5% 以上)。

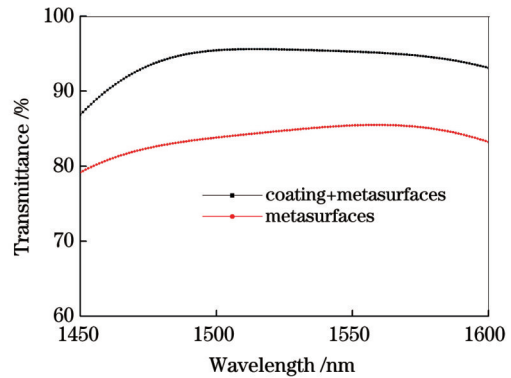


图 8 1450~1600 nm 波段有无光学薄膜的超构表面透镜的透过率

Fig. 8 Transmittance of metasurface lens with and without optical thin films at 1450~1600 nm wavelength

在红外波段,目前已知的透射型超构表面透镜的透过率在 70%~89% 之间<sup>[22-23]</sup>,低于所设计的超构表面透镜,说明所设计的超构表面结合光学薄膜结构是一种非常高效的提高透镜透过率的结构。聚焦效率通过聚焦的光能比总入射光能计算得到,从聚焦效率对比来看,有增透光学薄膜的超构表面透镜的聚焦效率远高于无增透膜时的聚焦效率,平均高 8.3% 以上。在

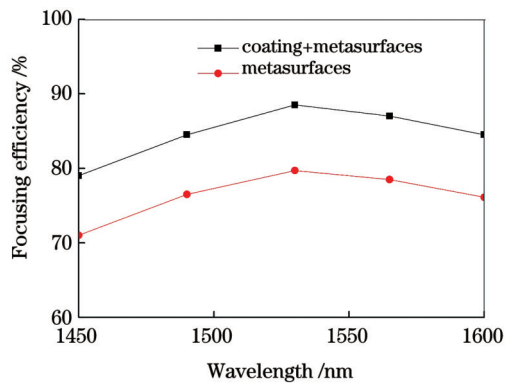


图9 不同波长处有无光学薄膜的超构表面透镜的聚焦效率  
Fig. 9 Focusing efficiency of metasurface lens with and without optical thin films at different wavelengths

1530 nm 波长处,聚焦效率最高达 88.5%。理论上合理优化超构表面聚焦效率最高可以达到峰值透过率 95.5%,说明增透光学薄膜对提高超构表面效率作用巨大。

## 4 结 论

总的来说,本研究首次提出了通过利用光学薄膜来提高超构表面效率的概念设想,研究了近红外波段超构表面透镜的特性,并基于超构表面附加功能性光学薄膜的性质研究了增透膜对超构表面透镜透过率和聚焦性能的影响。模拟计算结果表明:在 1450~1600 nm 波段,有光学增透膜的超构表面透镜的透过率远高于无光学增透膜时的透过率,平均高 10.5% 以上;从聚焦效率对比结果来看,有光学增透膜的超构表面透镜的聚焦效率比无增透膜时的聚焦效率平均高 8.3% 以上,聚焦效率最高达 88.5%。所提出的超构表面结合光学薄膜的设想有望解决超构表面普遍效率低的问题。该技术可以应用于平面透镜、涡旋相位片、全息相位片、偏振转换器和波长选择器等领域,为超构表面器件设计带来新的思路。

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## Study of High-Efficiency Metasurfaces Based on Optical Thin Films

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### Abstract

**Objective** The problem of low optical efficiency commonly exists on metasurfaces, which restricts their application and development. Although the efficiency of metasurfaces designed based on dielectric nanobricks structures is greatly improved compared to metal metasurfaces, the scattering and reflection losses of the unit structure are still relatively large. Metasurfaces are generally composed of high refractive index nanobricks to reduce their thickness and preparation process difficulty. Due to the high refractive index of the equivalent film layer on a high refractive index metasurfaces, it leads to significant interface reflection loss. In terms of improving the efficiency of metasurface devices, current research mainly focuses on improving the diffraction efficiency of metasurfaces and reducing scattering losses. However, there is no research focus on the reflection loss of metasurfaces currently, so it is necessary to study reducing the reflection loss of metasurfaces.

**Methods** We propose an efficient design scheme for metasurfaces based on optical thin film theory to solve the problem of interface reflection loss caused by the mismatch between the equivalent refractive index of the metasurfaces and the substrate, as well as the mismatch between the equivalent optical thickness of the metasurfaces and the wavelength. First, we design the metasurface lens. Then, based on the equivalent medium theory, the metasurfaces are equivalent to a layer of dielectric thin films and serve as the outermost layer of the multi-layer antireflection coating system, with the equivalent layer thickness being the height of the metasurfaces. Finally, the optical thin film theory is adopted to design the antireflection coating that matches the substrate and incident medium.

**Results and Discussions** We simulate the near-infrared broadband silicon nanobrick metasurface lens on the quartz substrate and compare it with the metasurfaces designed with optical thin films. The transmittance of the antireflection coating designed by the equivalent medium theory is much higher than that of the equivalent film layer on the metasurfaces, with an average transmittance of 12.4% higher (Fig. 4). Comparison is made between the light field distribution patterns of a metasurface lens without optical thin films and with optical thin films (the antireflection coating structure of optical thin films combined with a metasurface) at different wavelengths (1460, 1530, 1600 nm). It can be seen that the focal spot size and focal length of the two types of structured metasurfaces at the same wavelength are basically the same. In the case of optical thin films, the light intensity at the focal point is significantly higher than that without optical thin films, whereas the focal point position is not affected by the antireflection coating and remains unchanged. This indicates that optical thin films only increase the transmittance of the metasurfaces and have little effect on their focusing performance (Figs. 5–7). The transmittance curves in the 1450–1600 nm wavelength range and the focusing efficiency at 1450, 1490, 1530, 1565, 1600 nm wavelengths are simulated and calculated. From the transmittance curves, it can be seen that in the 1450–1600 nm wavelength range, the transmittance of the metasurface lens designed with optical thin films remains around 94.0%, with the highest peak reaching 95.5%, which is much higher than that of metasurface without optical thin films, with an average increase of more than 10.5% (Fig. 8 and Fig. 9). The results of simulation calculations indicate that our proposed idea of combining optical thin films with metasurfaces is reasonable and has the potential to be applied to the actual production of metasurfaces.

**Conclusions** We propose the concept of using optical thin films to improve the efficiency of metasurfaces. The characteristics of metasurface lens are studied in the near-infrared, and based on the properties of additional functional optical thin films on metasurfaces, the influence of the antireflection coating on the transmittance and focusing performance of metasurfaces are studied. Research has shown that combining the structure of optical thin films with the metasurfaces can significantly improve the optical efficiency of metasurfaces without affecting their optical properties. The idea of combining metasurfaces with the proposed optical thin films is expected to solve the problem of low efficiency of metasurfaces, bringing new ideas for the design of metasurface devices.

**Key words** metasurface; optical thin film; silicon nanobrick; transmittance