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Method for designing highly efficient composite transmission gratings

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We present and validate a new method for designing transmission gratings with high efficiency for the 1st diffraction order across the visible spectrum. The high efficiency is achieved by redirecting light to the 1st order via asymmetric composite elements, which scatter light in the same direction as the 1st diffraction order. By focusing on increasing the directional scattering of the grating elements, the design remains simple yet effective. As a result, the gratings are relatively easy to fabricate. Measurements of fabricated gratings show a relative increase of over 40% for a large part of the visible spectrum.

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1. INTRODUCTION

Gratings play an important role in many optical measurement devices, ranging from spectroscopy and telecommunications to laser technology. The efficiency of a grating, as measured in the amount of power that goes into a specific diffraction order divided by the input power, is an important property of a grating. Higher efficiencies mean that less input light is required for the same measurement.

A common method of increasing the grating efficiency for a specific order is by making use of a blazed grating. Due to the blazing, the light is refracted into one diffraction order. This is, however, not possible for gratings with a high line density due to internal reflections or shadowing effects.

To overcome this limitation, researchers develop diffraction gratings with multilayer systems [1], or complex geometries are created. For example, an effective blaze can be created by introducing a binary structure, which is further enhanced by adding a secondary binary layer on top that can be used to guide more of the light into the diffraction order [2]. A different method of increasing the efficiency of an effective blaze created by binary structures is the use of slanted elements [3]. Another approach is the use of resonant structures to create a phase profile comparable to that of a blazed structure [4,5].

In some cases, the efficiency can be increased to over 90%, as shown in the literature. In contrast, in this work, we present a grating that has a simple design and consequently is easily fabricated, while promoting a high efficiency for the 1st diffraction order across the entire visible spectrum.

Such a grating has been presented before [6], where the enhanced diffraction efficiency was explained by making a comparison with blazed gratings: the profile of the real part of the permittivity of a blazed grating and composite grating are comparable. In this paper, we will present an intuitive understanding of the increase in diffraction efficiency, which is based on the scattering characteristics of the grating elements.

Furthermore, we will present a method for the initial design and fabrication of these gratings, which is verified experimentally. Moreover, we will highlight the benefits of using semiconductor materials over metals for the design and fabrication of such gratings.

2. THEORY

In order to redirect light into one specific diffraction order, we will use the results of our earlier work [7]. We have shown that directional scattering can be achieved by nanoparticles, where the nanoparticles are composed of two different materials. This can be done either by placing the nanoparticle inside a medium with a refractive index between that of the two components or by using a lossy material for one of the components, which causes the light to scatter in a specific direction.

The explanation for this directionality is as follows: the two components of the nanoparticle will each scatter the light with a phase difference due to the difference of optical properties between the two materials. As a result, the total scattered field can be suppressed or enhanced in different directions.

Instead of considering a single nanoparticle, we can create grating lines following the same idea. By engineering a grating element that preferentially scatters in the same direction as a diffraction order of the total grating, the grating efficiency can be enhanced significantly. Moreover, as we have shown in our previous paper, the fabrication process is fairly simple.

We will start with the design of a standard rectangular grating fully made of glass (with a refractive index of 1.53 for both the

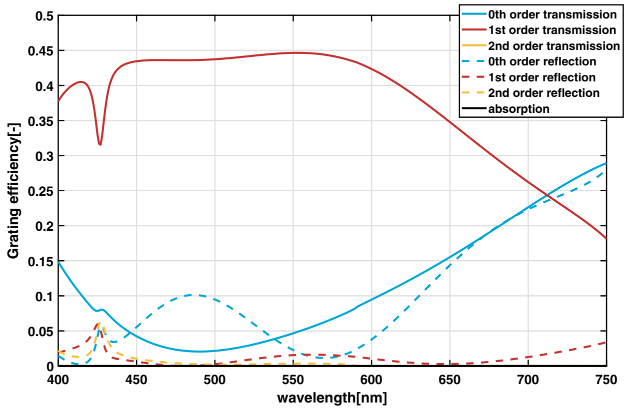

Fig. 1. Grating diffraction efficiency and absorption of a rectangular grating made of glass, when a plane wave—polarized along the grating lines—is incident perpendicular to the surface. The grating has a pitch of $p = 775$ nm, and the grating elements have a height of $h = 520$ nm and a width of $w = 260$ nm.

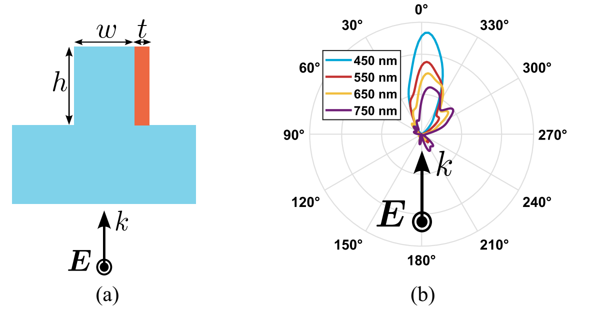

Fig. 2. (a) Geometry of a single grating element with height h, width w, and metal thickness t and (b) resulting scattering pattern when a plane wave polarized along the grating lines is incident from the bottom of an element composed of fused silica and gold for some wavelengths in the visible spectrum.

grating lines and the substrate), where we use FEM simulations to find an initial design. The aim is to get most of the energy coming into the grating to be transmitted into the 1st and −1st diffraction orders. The result is a rectangular grating optimized for the visible spectrum with a pitch of $p = 775$ nm, a height of $h = 520$ nm, and a width of $w = 260$ nm. For now, the grating is symmetric, resulting in an overlap of the efficiencies of the negative and positive diffraction orders. The calculated diffraction efficiencies for the different orders and the absorption are shown in Fig. 1.

It can be seen that the 0th transmission order has been suppressed to a minimum at a wavelength of 490 nm. However, there is still a significant contribution by the 0th order reflection, resulting in a maximum efficiency of about 43% for the −1st and 1st orders. As the wavelength increases, the efficiency drops as a result of increased 0th order transmission and reflection. There is no absorption because the only material used is glass (which is assumed to be transparent for the entire considered spectrum).

Now that the initial shape of the grating elements is known, we can change it by adding a second material to the side of the elements so the scattering becomes anisotropic. The ratio between the volumes of each material is determined by the permittivity functions, as it is important that the total magnitude of light scattered by each material is comparable in order for the scattering to become anisotropic. To allow for directional scattering inside air, a material with a complex permittivity has to be used. Metals are an obvious choice, as they are compatible with many nanofabrication technologies and are lossy in the visible part of the spectrum.

The scattering by a single composite grating element is determined using FEM simulations; details on the simulation can be found in Supplement 1. The geometry used in the simulations is shown in Fig. 2(a), and the results for some selected wavelengths are shown in Fig. 2(b). In this example, a layer of $t = 40$ nm gold is added to the side of a grating element made of fused silica (refractive index of 1.46) with $h = 550$ nm and $w = 260$ nm on a substrate of the same material. It can be seen that the scattered field from an incident plane wave polarized along the grating lines has become asymmetric, which will later result in an improved grating efficiency for the order that coincides with the direction of the scattered light. The effect of adding more grating elements together is shown in Fig. 3, for 2, 5, and 10 elements.

It should be noted that, for a wave which is polarized perpendicular to the grating lines, only a slight increase in the efficiency of the −1st order versus the 1st order can be expected as a consequence of the scattering by the individual grating elements.

Next, the full grating is simulated using composite grating elements by introducing periodic boundary conditions. From here, the grating shape is further optimized by changing its height, width, and metal thickness to account for the interaction

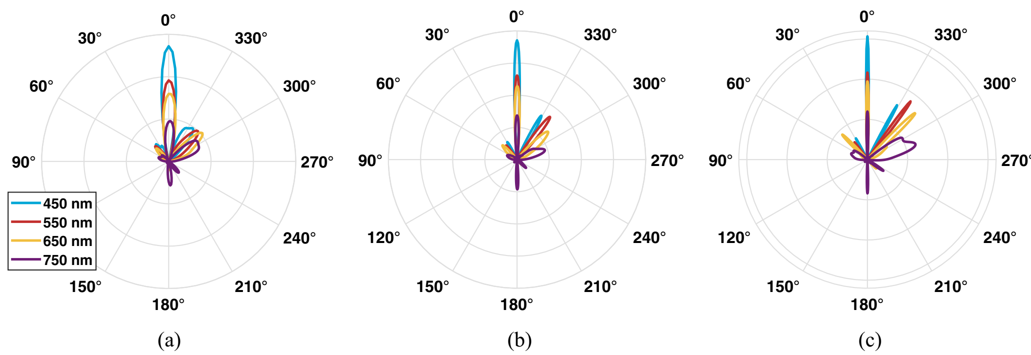

Fig. 3. Scattering pattern of (a) 2, (b) 5, and (c) 10 elements composed of fused silica and gold for various wavelengths in the visible spectrum, when a plane wave polarized along the grating lines is incident from the bottom.

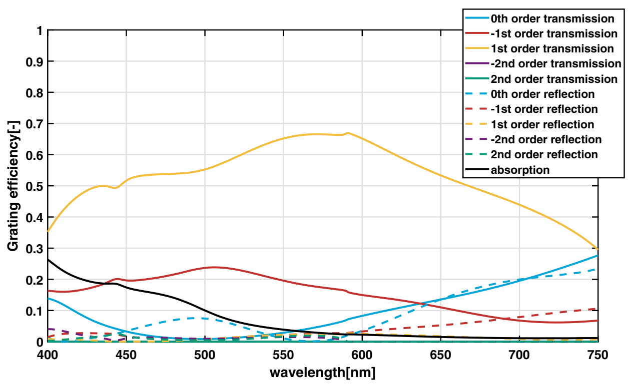

Fig. 4. Grating diffraction efficiency and absorption of a rectangular composite grating made from fused silica and gold, when a plane wave—polarized along the grating lines—is incident perpendicular to the surface. The grating has a pitch of $p = 775$ nm, the fused silica part of the elements has a height of $h = 520$ nm and a width of $w = 260$ nm, and the layer of gold has a thickness of $t = 40$ nm.

between the grating elements to achieve the highest possible grating efficiency. Using gold as a second material, a grating efficiency for the 1st order of >60% can be achieved for the 1st diffraction order, as shown in Fig. 4.

As we will show later in this paper, the measured diffraction efficiency does not reach what is predicted in simulations. This is due to the modeling of the ultra-thin metal film. At such dimensions, the metal films are not smooth but are made up of many small islands. The consequence of this is that the electrons scatter on the surface of these islands, changing the response of the electrons to an incident electromagnetic wave and increasing the absorption [8]. Furthermore, the rough geometry increases the diffuse scattering, which does not contribute to the diffraction orders.

Instead of using metal, we can consider the use of semiconductor materials to limit the amount of light that is absorbed by the grating. These materials do not have such a large absolute permittivity, and thus allow more of the material to be deposited while maintaining the balance between the amount of fused silica and semiconductor material. In this case, fewer (or no) small islands are created, and thus less light is lost due to absorption and diffuse scattering.

3. FABRICATION

To determine the practical performance of the proposed composite gratings, gratings of 5 by 5 mm were fabricated through a combination of e-beam lithography and etching steps.

First, 25.4 mm fused silica wafers were coated with a 25 nm layer of titanium using physical vapor deposition to allow for use with the e-beam pattern generator. Next, a negative resist (ARN-7520.17 NEW Allresist) was spin-coated onto the wafers. Using an e-beam pattern generator, the grating designs were transferred onto the resist. Afterward, the resist was developed using the MF-322 developer.

The patterns were then transferred into the fused silica wafer using reactive ion etching, where CHF_3 gas was used to etch into the fused silica. During this etching process, the deposited titanium layer is also completely etched away. The height of the grating elements was measured using a profilometer.

As a next step, a metal is evaporated onto the grating elements at an angle; different commonly found metals (Pt, Au, Al, Ag, and Ti) were used to determine the material that had the best performance. The angle is chosen such that no metal

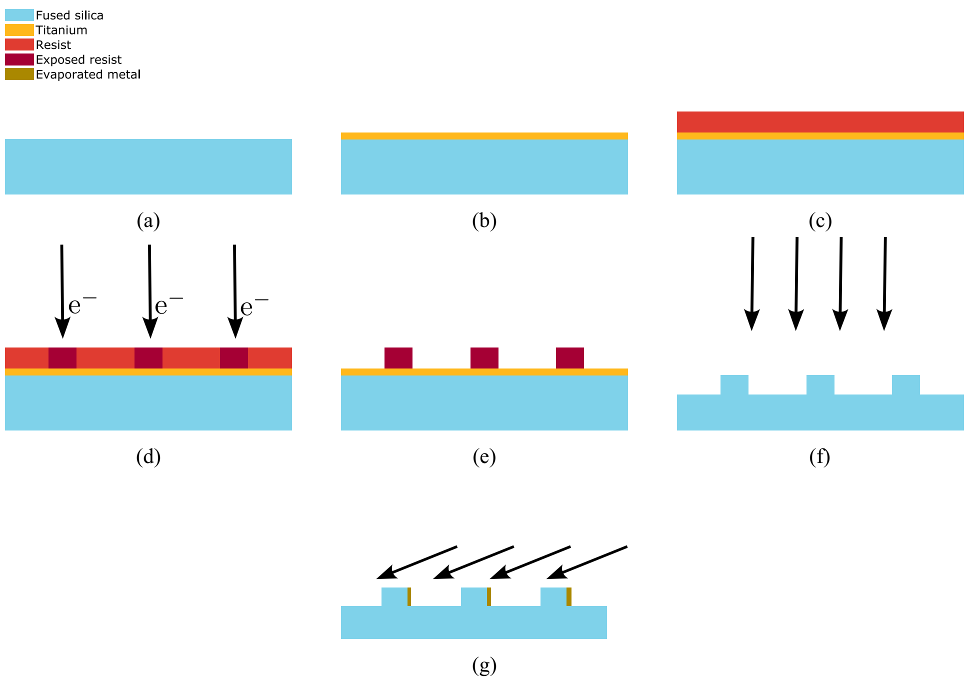

Fig. 5. Schematic representation of the fabrication process. (a) Fused silica wafers were (b) coated with titanium. Next, the samples were (c) coated with a negative resist and (d) exposed by the e-beam. (e) The grating pattern was developed and (f) transferred into the fused silica through reactive ion etching. (g) Finally, a metal was evaporated at an angle on the side of the grating elements.

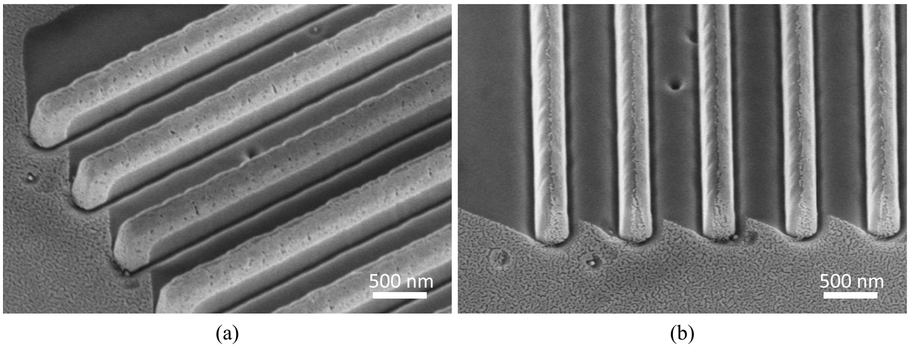

Fig. 6. (a) SEM image of a fused silica and platinum composite diffraction grating as seen from the side. The deposited platinum can be seen on the left side of the silica grating elements. The shadowing effect that the grating lines have on the deposited platinum is clearly visible. (b) Same grating as seen from the top, where the right side of the grating lines is covered by platinum.

is deposited between the grating lines. The amount of metal deposited can be controlled via the evaporation time and by further increasing the deposition angle. The fabrication steps are schematically shown in Fig. 5. More details of the full fabrication process can be found in Supplement 1.

An SEM image of the fabricated composite grating, made with platinum, can be seen in Fig. 6. It can be seen that the grating lines are covered by a metal film, which is also visible by the substrate next to the grating lines. Due to the angle of the metal deposition, a shadow is created by the grating lines where no metal is deposited. Part of the shadow can be seen extending over to the next grating line. For the last grating line at the top, the shadow on the substrate where no metal is deposited can clearly be seen.

4. MEASUREMENTS

Measurements were performed using a goniometer setup, as shown in Fig. 7. It allows for the measurement of the light intensity at different angles, while the lens capturing the light remains perpendicular to the diffracted light.

Light from a stabilized broadband tungsten-halogen source (Thorlabs SLS201/M 360–2600 nm) was coupled into an optical fiber. This fiber was coupled to a collimator to illuminate the grating sample. After the fiber collimator, a linear polarization filter and diaphragm were placed. This way, the direction of polarization and spot size on the grating could be controlled. The light is then collected using another fiber collimator. This collimator was mounted on a rotational stage, such that it could rotate around the sample and capture all the transmitted diffraction orders.

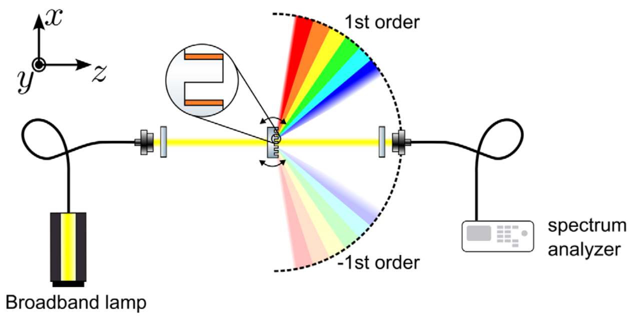

Fig. 7. Goniometer setup to measure the diffraction efficiency of the fabricated composite diffraction gratings.

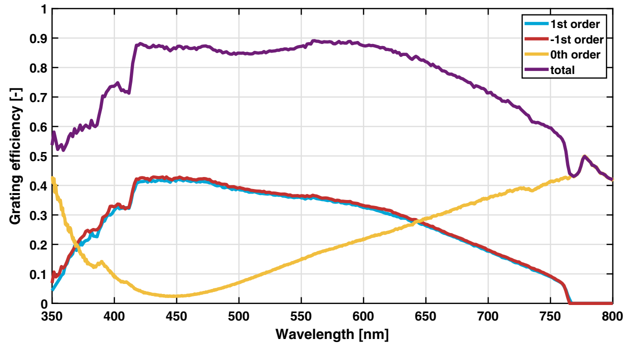

Fig. 8. Measured grating efficiency for the transmitted diffraction orders of a rectangular silica grating with height $h = 560$ nm, width $w = 260$ nm, and pitch $p = 775$ nm. Light is incident normal to the grating and polarized along the grating lines.

The sample was mounted on several stages: a linear stage to move along the z direction, to make sure the sample is in the center of the circle of the collection collimator; a rotational stage such that the sample could be rotated along the y axis, to change the angle of incidence of the light; and a rotational stage that could rotate the sample around the z axis to make sure the diffraction orders are aligned with the collection collimator. Light from the fiber collimator was sent to a spectrometer, allowing us to extract the diffraction efficiency.

To get a baseline for the grating measurements, the different gratings were first measured before the metal deposition step. The results of such a measurement are shown in Fig. 8. We can see that the resulting efficiency graph is similar to that of the simulations (Fig. 1).

The drop in transmission for the lower wavelengths is likely due to diffuse scattering caused by the surface roughness of the produced grating. For the longer wavelengths, reflection is the source of the reduced total transmission. The dip seen in the total transmission at around 760 nm is due to the diffracted light having such a high angle that it is blocked by the sample holder. Further differences with respect to simulations can be attributed to inaccuracies in the fabrication of the grating, which could be resolved by optimizing the fabrication process.

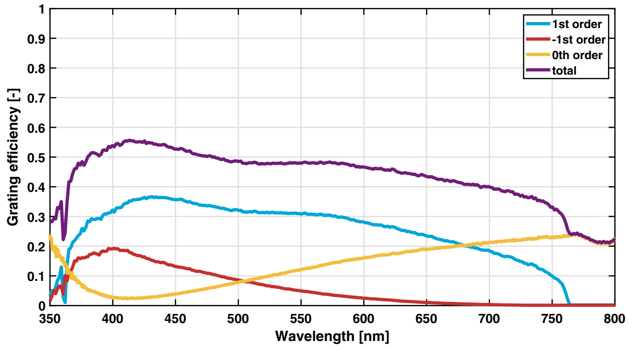

Fig. 9. Measured grating efficiency for the transmitted diffraction orders of a rectangular composite grating made with height $h = 560$ nm, width $w = 260$ nm, and pitch $p = 775$ nm, and a layer of $t = 15$ nm of titanium deposited at an angle of 60 deg. Light is incident normal to the grating and polarized along the grating lines.

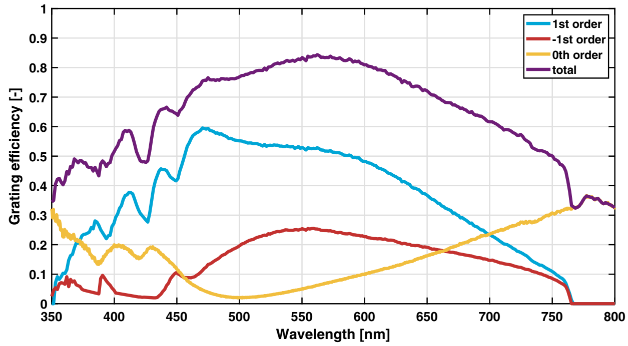

Fig. 10. Measured grating efficiency for the transmitted diffraction orders of a rectangular composite grating after annealing in a nitrogen environment at 400°C made with height $h = 560$ nm, width $w = 260$ nm, and pitch $p = 775$ nm, and a layer of $t = 15$ nm of titanium deposited at an angle of 60 deg. Light is incident normal to the grating and polarized along the grating lines.

After the deposition of a metal, a clear splitting between the 1st and −1st transmitted diffraction orders can be observed. However, much more absorption and diffuse scattering can be observed than predicted by the simulations. An example is shown in Fig. 9, where titanium was used. Measurements of gratings where platinum, gold, or silver were used can be found in Supplement 1.

As a result, the permittivity function used for the metals in the simulations is not accurate anymore. In general, this results in an increase in absorption for optical frequencies; the same is observed in our experiments. The difficulty in this is that the permittivity is dependent on the layer thickness and fabrication process, making modeling difficult. Therefore, we suggest an empirical approach, where an initial design is generated through modeling and further optimizations are done by changing the fabrication process.

The amount of material to be added to a standard glass grating can easily be found, as there will be an optimum in the case that the components of a grating element scatter a similar amount of light. From there, the fabrication process should be optimized so that the grating scatterers as little diffuse light as possible by making the added material as smooth as possible.

As we have mentioned before, using a semiconductor material may alleviate some of these issues. In our experiments, we have created the semiconductor material by annealing deposited titanium inside a nitrogen environment at 400°C so that titanium nitrate (TiN) is formed [9]. No simulations have been done for this case, as the TiN would be subject to the same change in permittivity. The samples were measured, and based on the measurements, the amount of Ti used was changed to optimize the efficiency of the 1st diffraction order. The results of the best-performing sample are shown in Fig. 10; others can be found in Supplement 1.

It can be seen that the amount of light in the transmitted order is hugely increased due to the annealing process. Furthermore, the efficiency of the 1st diffraction order is also increased, almost reaching 60% at a wavelength of 470 nm. This is equal to a relative diffraction efficiency increase of the 1st order of over 40% for a large part of the visible spectrum compared to a bare fused silica grating. More improvements are clearly possible, as the amount of light in the transmitted orders does not even reach 80% for most of the visible spectrum.

5. CONCLUSION

In this paper, we have shown that composite grating elements, which scatter the incident light to one side, can be used to create a grating with high diffraction efficiency over the entire visible spectrum. A method was laid out for the initial design of such gratings, and these gratings were fabricated using simple nanofabrication techniques.

By adding the right amount of material with a complex permittivity to the side of normal fused silica grating lines, the scatter pattern of the grating element can be changed. Through this change, more light can be directed in the same direction as a diffraction order, resulting in an increase in diffraction efficiency for that order. Semiconductor materials seem to be a better choice over metals, as this results in less absorption and diffuse scattering.

We have experimentally demonstrated that a composite grating with a relative efficiency increase of over 40% for a large part of the visible spectrum can be achieved with very little optimization of the grating design. We imagine that further optimizations are possible to increase the efficiency even more.

The simplicity of the fabrication of such gratings makes it possible for these gratings to be produced at a large scale and low cost. This would make it possible for these kinds of high-efficiency gratings for a large bandwidth to become widely available.

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Disclosures. The authors declare no conflicts of interest.

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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