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Omnidirectional wavelength selective emitters/absorbers based on dielectric-filled anti-reflection coated two-dimensional metallic photonic crystals

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ABSTRACT

We demonstrate designs of dielectric-filled anti-reflection coated (ARC) two-dimensional (2D) metallic photonic crystals (MPhCs) capable of omnidirectional, polarization insensitive, wavelength selective emission/absorption. Up to 26% improvement in hemispherically averaged emittance/absorptance below the cutoff wavelength is observed for optimized hafnium oxide filled 2D tantalum (Ta) PhCs over the unfilled 2D Ta PhCs. The optimized designs possess high hemispherically averaged emittance/absorptance of 0.86 at wavelengths below the cutoff wavelength and low hemispherically averaged emittance/absorptance of 0.12 at wavelengths above the cutoff wavelength, which is extremely promising for applications such as thermophotovoltaic energy conversion, solar absorption, and infrared spectroscopy.

Keywords: Photonic crystals, selective emitter/absorber, thermal emission, nanophotonics, high-temperature.

1. INTRODUCTION

Naturally occurring materials usually exhibit thermal emission profiles that are broadband, and have a magnitude far weaker compared to the ideal blackbody. This is inefficient for many applications, for instance as an infrared source in sensing applications,1,2 as an emitter in thermophotovoltaic (TPV) energy conversion,3,4 and as a solar absorber.5,6 For many of these applications, it is desirable to accurately control thermal radiation such that thermal emission occurs only in certain wavelength ranges over an optimum angular spread. For instance, TPV energy conversion systems benefit from the use of omnidirectional polarization insensitive selective emitters,4 while solar absorbers that possess angularly selective absorbance are more efficient.6

To-date, various one-dimensional (1D),2,7–9 2D,10–17 and 3D18–20 periodic structures have been investigated both theoretically and experimentally in order to achieve accurate control of thermal radiation. The first class of these relies on excitation of surface phonon-polaritons,7 surface plasmon-polaritons,2,11,21 and localized plasmon resonances.22 These mechanisms usually result in very sharp and narrow thermal emission linewidths with respect to wavelength, and can be designed to emit over restricted,7,21 or wide polar angles.10,22 Thermal emission can also be enhanced by coupling to magnetic polaritons to obtain narrowband emission over wide polar angles.23

In certain applications, for instance as a selective emitter in TPV energy conversion systems, it is more advantageous to possess broader emission bandwidth such that high emittance is retained at wavelengths \( \lambda \) smaller than a particular cutoff wavelength \( \lambda_{\text{cut}} \) while maintaining ultra-low emittance at \( \lambda > \lambda_{\text{cut}} \) over all exitance angles and polarizations. In this respect, metamaterial designs based on metal dielectric stacks7 and 2D metallic pyramid arrays15 show great promise.

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However, they are difficult to fabricate, and have not been experimentally demonstrated at high temperatures under extended operation. Here, we present a simpler approach based on dielectric-filled anti-reflection coated (ARC) 2D metallic photonic crystals (MPhCs) to obtain omnidirectional polarization insensitive wavelength selective thermal emission.

2. DESIGN AND OPTIMIZATION

The traditional unfilled 2D MPhCs consists of a square array of cylindrical holes with period $a$, radius $r$, and depth $d$ etched onto a metallic substrate, as shown in Figure 1(a).\textsuperscript{13,17} This design achieves selective emission by relying on cavity resonances, whereby $\lambda_{\text{cut}}$ is determined by the fundamental cavity resonance mode. When the absorptive and radiative rates of the MPhC’s cavity resonances are matched, i.e. $Q$-matched, it is possible to achieve near-blackbody emittance $\varepsilon$ at $\lambda < \lambda_{\text{cut}}$ as well as emittance almost as low as a polished metal at $\lambda > \lambda_{\text{cut}}$ with a sharp cutoff separating the two regimes.\textsuperscript{17,24} This approach is general, and therefore applicable to any highly reflective metallic material of choice, for instance silver, platinum, tungsten, etc. In this investigation, tantalum (Ta) is our material of choice given its ultra-low emittance at $\lambda > \lambda_{\text{cut}}$, and high temperature stability. Furthermore, 2D Ta PhCs have been demonstrated at scale,\textsuperscript{25} and have been shown to be thermally stable at high temperatures under high vacuum conditions.\textsuperscript{26}

While $Q$-matching can successfully be used to quickly obtain designs with high emittance at $\lambda < \lambda_{\text{cut}}$, it is not a globally optimum design as it is impossible to satisfy $Q$-matching conditions for all higher order modes simultaneously, which is important in broadening the bandwidth for maximum emittance at $\lambda < \lambda_{\text{cut}}$. In addition, the optimization problem is highly non-convex marked by a large number of local optima. Hence, non-linear global optimization methods were used to uncover the optimum $a$, $r$, and $d$ of the 2D Ta PhC that would possess maximum emittance at $\lambda < \lambda_{\text{cut}}$ as local search algorithms may potentially get trapped in a localized peak.\textsuperscript{27} The global optimum was found via the multi-level single-linkage (MLSL) method, which executes a quasi-random low-discrepancy sequence (LDS) of local searches using constrained optimization by linear approximation (COBYLA).\textsuperscript{28,29} We have also verified that other global search algorithms, such as the controlled random search (CRS) algorithm,\textsuperscript{30} yielded similar results. The global optimization routines were implemented via NLOpt, a free software packaged developed at MIT that allows comparison between various global optimization algorithms.\textsuperscript{31} Note that in all optimization routines, the design provided by $Q$-matching of the fundamental mode was used as the initial estimate. In addition, the following constraints were implemented: $a-2r < 100\text{nm}$ to ensure integrity of sidewalls; $d < 8.50\mu\text{m}$ based on fabrication limits using an SF$_6$ based Bosch deep reactive ion etching (DRIE) process.\textsuperscript{25}

![Figure 1: (a) Traditional unfilled two-dimensional metallic photonic crystal (2D MPhC) with period $a$, radius $r$, and depth $d$. (b) Dielectric-filled 2D MPhC with additional anti-reflection coating (ARC) of the same dielectric material of thickness $t$. $\theta$ and $\phi$ respectively denotes the polar and azimuthal angle.](http://proceedings.spiedigitallibrary.org/conferences/9170X-2/91700X-2)
The emittance of the 2D Ta PhC can easily be determined via finite-difference time-domain (FDTD) numerical methods\textsuperscript{32} coupled with the Lorentz–Drude model fitted to measured room and elevated temperature emittance\textsuperscript{33} to capture the optical dispersion of Ta. However, high memory requirements and slow computational speed of FDTD methods limit its application, particularly in determining the globally optimum design for a particular application. Thus, to obtain quicker estimates, we utilized rigorous coupled wave analysis (RCWA) methods.\textsuperscript{34} To ensure accuracy, the number of Fourier components were doubled until the results converged. We have also verified that FDTD methods agree very well with RCWA formulations based on both polarization decomposition and normalized vector bases when more than 320 Fourier expansion orders were used.

Figure 2(a) shows the emittance as a function of wavelength and polar angle of the traditional unfilled 2D Ta PhC optimized for maximum emittance at $\lambda < \lambda_{\text{cut}}$. As can be seen, the average emittance at $\lambda < \lambda_{\text{cut}}$ is high at near-normal incidence polar angles. However, as the polar angle increases, the average emittance at $\lambda < \lambda_{\text{cut}}$ falls significantly. The reason for this is the presence of diffraction losses, which is governed by the grating equation:

$$a(\sin \theta_i + \sin \theta_m) = m\lambda, \quad m = \pm 1, \pm 2, \pm 3, \ldots \quad (1)$$

where $\theta_i$ is the angle of incidence, and $\theta_m$ is the angle where the $m$-th order diffraction exists. The onset of diffraction occurs when $m = 1$ and $\theta_m = 90^\circ$. Thus, for radiation with a specific wavelength, diffraction sets in when $\theta_i$ is larger than the cutoff angle given by:

$$\theta_d = \sin^{-1}\left(\frac{\lambda}{a} - 1\right) \quad (2)$$

Above this diffraction threshold, there are more channels to couple into, resulting in a smaller radiative $Q$. The initial match with the absorptive $Q$ is thus lost, resulting in severe reduction in average emittance at $\lambda < \lambda_{\text{cut}}$. This effect is clearly observed in Figure 2(a) as indicated by the white lines, which are the diffraction thresholds as determined by Equation (2).
In order to reduce diffraction losses, $\theta_d$ has to be increased by reducing $a$ as much as possible. A simple solution to reduce $a$ is filling the cylindrical cavities with an appropriate dielectric, thereby increasing $\theta_d$ by virtue of a reduced $r$, $d$, and hence $a$ to obtain the same $\lambda_{cut}$ due to a reduced effective wavelength by a factor of $n$ in dielectrics.\textsuperscript{15} In addition, we consider an additional coating of the same dielectric with thickness $t$ that enhances the emittance at $\lambda < \lambda_{cut}$ by functioning as an ARC. In this investigation, we have selected hafnium oxide (HfO$_2$) because of its transparency in the visible and infrared (IR) region, its compatible thermal expansion coefficient, and its high melting point. HfO$_2$ can also be easily deposited via atomic layer deposition (ALD),\textsuperscript{26} and sol-gel deposition methods.\textsuperscript{36} Furthermore, the HfO$_2$ layer promotes stable operation at high temperatures by preventing debilitating chemical reactions that attack the top surface of Ta, and preventing geometry deformation due to surface diffusion.\textsuperscript{26,36} In our numerical simulations, the refractive index $n$ of HfO$_2$ was assumed to be 1.9 for $0.5\mu m < \lambda < 5.0\mu m$, which is consistent with results reported in literature,\textsuperscript{37} and our measurements of HfO$_2$ thin films deposited via ALD (Cambridge NanoTech Savannah).

Results of non-linear global optimization routines applied to HfO$_2$-filled ARC 2D Ta PhC for $\lambda_{cut}$ of 2$\mu m$ are shown in Figure 2(b). As can be seen, the optimized HfO$_2$-filled ARC 2D Ta PhC more closely approaches the ideal cutoff emitter (hemispherically averaged emittance of 1 at $\lambda < \lambda_{cut}$ and hemispherically averaged emittance of 0 at $\lambda > \lambda_{cut}$); the emittance is essentially unchanged up to $\theta = 40^\circ$, and is $> 0.8$ for $\theta > 70^\circ$, a significant improvement compared to the traditional unfilled 2D Ta PhC. The HfO$_2$-filled ARC 2D Ta PhC can also be easily optimized for different $\lambda_{cut}$\textsuperscript{8} as illustrated in Figure 3(a) using the aforementioned optimization methods. In addition, other suitable dielectric materials could be used, for instance silicon dioxide (SiO$_2$) which has $n \approx 1.45$.\textsuperscript{38} As shown in Figure 3(b), optimized HfO$_2$-filled and SiO$_2$-filled ARC 2D Ta PhCs show very similar performance. However, when using dielectrics with smaller $n$, larger $a$, $r$, $d$, and $t$ are necessary to achieve optimal performance as shown in Table 1. The eventual choice will nevertheless depend more on thermal stability, ease of fabrication, and overall cost.

<table>
<thead>
<tr>
<th>Dielectric</th>
<th>Period, $a$ ($\mu m$)</th>
<th>Depth, $d$ ($\mu m$)</th>
<th>Radius, $r$ ($\mu m$)</th>
<th>Thickness, $t$ ($\mu m$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air ($n = 1$)</td>
<td>1.16</td>
<td>8.50</td>
<td>0.53</td>
<td>N/A</td>
</tr>
<tr>
<td>SiO$_2$ ($n = 1.45$)</td>
<td>0.80</td>
<td>6.28</td>
<td>0.35</td>
<td>125</td>
</tr>
<tr>
<td>HfO$_2$ ($n = 1.90$)</td>
<td>0.57</td>
<td>4.31</td>
<td>0.23</td>
<td>78</td>
</tr>
</tbody>
</table>

Figure 3: (a) Optimized HfO$_2$-filled ARC 2D Ta PhC designs for $\lambda_{cut} = 1.7\mu m$ ($a = 0.49\mu m$, $r = 0.19\mu m$, $d = 3.62\mu m$, $t = 63nm$), $\lambda_{cut} = 2.0\mu m$ ($a = 0.57\mu m$, $r = 0.23\mu m$, $d = 4.31\mu m$, $t = 78nm$), and $\lambda_{cut} = 2.3\mu m$ ($a = 0.64\mu m$, $r = 0.27\mu m$, $d = 5.28\mu m$, $t = 80nm$). $\lambda_{cut}$ can easily be shifted by altering $a$, $r$, $d$, and $t$, and further fine-tuned using global non-linear optimization routines. (b) Comparison between optimized HfO$_2$-filled ($n \approx 1.9$) and SiO$_2$-filled ($n \approx 1.45$) ARC 2D Ta PhCs for $\lambda_{cut} = 2.0\mu m$. Similar performance is obtained, albeit at a penalty of larger $a$, $r$, $d$, and $t$ when using dielectrics with smaller $n$ as shown in Table 1.
3. ANALYSIS: THERMOPHOTOVOLTAIC ENERGY CONVERSION

In this section, we analyze the performance of optimized HfO$_2$-filled ARC 2D Ta PhCs as a selective emitter in an InGaAsSb TPV energy conversion system. Using the numerical model outlined in Ref. 4, we can determine the following figure of merit for optimization purposes:

\[
FOM = x \eta_{TPV} + (1 - x) \frac{J_{elec}^{PhC}}{J_{elec}^{BB}}
\]

where $\eta_{TPV}$ is the radiative heat-to-electricity efficiency and $J_{elec}^{PhC} / J_{elec}^{BB}$ captures the TPV system power density performance of the optimized PhC selective emitter compared to the blackbody, and $x \in [0,1]$ is the weighting given to $\eta_{TPV}$. Here, we are mainly concerned on obtaining the highest $\eta_{TPV}$ possible, thus $x = 0.9$ was used. Results of the optimization of an indium gallium arsenide antimonide (InGaAsSb) TPV energy conversion system for a temperature of 1250K with a view factor of 0.99 (achievable with 100mm X 100mm flat plate geometry with emitter-TPV cell separation of 500$\mu$m) are shown in Table 2. Note that high temperature optical constants of Ta were used in the simulations. Clearly, when operated at higher temperatures, a much smaller $d$ is sufficient for optimum performance due to increased intrinsic absorption of Ta, and is thus easier to fabricate.

Table 2: Comparison of radiant heat-to-electricity efficiency $\eta_{TPV}$ and electrical power density generated $J_{elec}$ between a greybody emitter ($\epsilon = 0.9$), optimized unfilled 2D Ta PhC ($a = 1.23\mu$m, $r = 0.57\mu$m, $d = 4.00\mu$m), and optimized HfO$_2$-filled ARC 2D Ta PhC ($a = 0.73\mu$m, $r = 0.22\mu$m, $d = 0.75\mu$m, $t = 146$ nm) in indium gallium arsenide antimonide (InGaAsSb) thermophotovoltaic (TPV) energy conversion systems at temperature of 1250 K and view factor of 0.99 (achievable with 100mm X 100mm flat plate geometry with emitter-TPV cell separation of 500$\mu$m).

<table>
<thead>
<tr>
<th>Emitter</th>
<th>Filter</th>
<th>$\eta_{TPV}$ (%)</th>
<th>$J_{elec}$ (W/cm$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Greybody ($\epsilon = 0.9$)</td>
<td>N/A</td>
<td>6.38</td>
<td>0.781</td>
</tr>
<tr>
<td>Optimized 2D Ta PhC</td>
<td>N/A</td>
<td>12.03</td>
<td>0.621</td>
</tr>
<tr>
<td>Optimized HfO$_2$-filled ARC 2D Ta PhC</td>
<td>N/A</td>
<td>12.71</td>
<td>0.713</td>
</tr>
<tr>
<td>Greybody ($\epsilon = 0.9$)</td>
<td>10 layer Si/SiO$_2$</td>
<td>12.52</td>
<td>0.700</td>
</tr>
<tr>
<td>Optimized 2D Ta PhC</td>
<td>10 layer Si/SiO$_2$</td>
<td>18.31</td>
<td>0.568</td>
</tr>
<tr>
<td>Optimized HfO$_2$-filled ARC 2D Ta PhC</td>
<td>10 layer Si/SiO$_2$</td>
<td>19.34</td>
<td>0.646</td>
</tr>
<tr>
<td>Greybody ($\epsilon = 0.9$)</td>
<td>Rugate Tandem Filter</td>
<td>23.44</td>
<td>0.726</td>
</tr>
<tr>
<td>Optimized 2D Ta PhC</td>
<td>Rugate Tandem Filter</td>
<td>23.68</td>
<td>0.588</td>
</tr>
<tr>
<td>Optimized HfO$_2$-filled ARC 2D Ta PhC</td>
<td>Rugate Tandem Filter</td>
<td>23.76</td>
<td>0.671</td>
</tr>
</tbody>
</table>

In TPV systems without a cold-side filter, the optimized HfO$_2$ ARC 2D Ta PhC enables up to 99% and 6% relative improvement in $\eta_{TPV}$ over the greybody emitter ($\epsilon = 0.9$) and the optimized unfilled 2D Ta PhC respectively. More importantly, up to 15% relative improvement is seen in $J_{elec}$ with the optimized HfO$_2$-filled ARC 2D Ta PhC compared to the unfilled 2D Ta PhC due to 26% relative improvement in hemispherically averaged emittance at $\lambda < \lambda_{cut}$. The improved electrical power density is especially vital in many portable power applications where power generated per kilogram of weight (W/kg) is the primary figure of merit.

It is also interesting to compare the performance when coupled with notable experimentally realized reflective spectral control devices, namely the 10 layer Si/SiO$_2$ filter$^{39}$ or the Rugate tandem filter$^{40}$. As can be seen, the improvement in $J_{elec}$ is observed even when either filter is included. However, as better filters are used (e.g. Rugate tandem filter), the improvement in $\eta_{TPV}$ from implementing MPhCs over a greybody becomes insignificant. Nevertheless, it is also
important to note that Rugate tandem filters are extremely costly and difficult to fabricate, given the sheer number of layers (> 50 layers) and the specialty materials used (antimony selenide, yttrium fluoride, and heavily doped indium phosphide arsenide). When the much more practical 10 layer Si/SiO₂ filter stack is used instead, the 2D Ta PhC selective emitter enables > 45% relative improvement over the greybody emitter. Additionally, the performance of the optimized 2D Ta PhC selective emitter based TPV system is improved by > 50% when the simple 10 layer Si/SiO₂ filter is used. Ultimately, the optimum combination would depend on cost and design goals of a specific application.

4. CONCLUSIONS

In summary, we have demonstrated optimized designs of dielectric-filled ARC 2D MPhCs for broadband wavelength selective emission. Using non-linear global optimization methods, optimized HfO₂-filled ARC 2D MPhC designs exhibiting up to 26% improvement in hemispherically averaged emittance at $\lambda < \lambda_{\text{cut}}$ over the unfilled 2D MPhC are demonstrated. The optimized designs possess high hemispherically averaged emittance of 0.86 at $\lambda < \lambda_{\text{cut}}$ and low hemispherically averaged emittance of 0.12 at $\lambda > \lambda_{\text{cut}}$ over all polar angles and polarizations at $T < 100$°C, whereby $\lambda_{\text{cut}}$ can easily be shifted and optimized via non-linear global optimization tools. At high temperatures ($T \approx 1250$K), the hemispherically averaged emittance at $\lambda > \lambda_{\text{cut}}$ increases to 0.26 due to primarily the reduction in DC-conductivity, hence making the metal more lossy at long wavelengths. This limitation is inherent to all metal based selective emitters, and is thus unavoidable. Regardless, the dielectric-filled ARC 2D MPhC design drastically reduces diffraction losses at $\lambda < \lambda_{\text{cut}}$ compared to the unfilled 2D MPhC. This translates into $\approx 15\%$ improvement in generated electrical power density for TPV systems, which is vital in many portable power applications. These designs also provide the platform necessary for many applications, ranging from solar absorbers for solar thermal applications, to near- to mid-IR radiation sources for IR spectroscopy. Our current work on realizing the dielectric-filled ARC 2D MPhCs experimentally has proven promising thus far, and will be presented in future publications.

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