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# Improved Omnidirectional 2D Photonic Crystal Selective Emitter for Thermophotovoltaics

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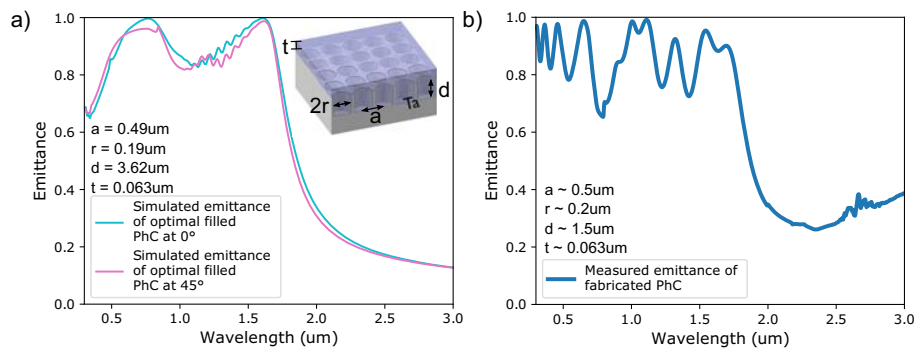
**Abstract.** Hafnia-filled, two dimensional (2D) tantalum (Ta) photonic crystals (PhCs) are promising emitters for high performance thermophotovoltaic (TPV) systems because they enable, for a wide range of incidence angles, efficient spectral tailoring of thermal radiation. However, fabricating these PhCs to the required tolerances has proven to be a challenging task. In this paper, we use both focused ion beam (FIB) imaging and simulations to investigate the effects of fabrication imperfections on the emittance of a fabricated hafnia-filled PhC and to identify critical geometric features that drive the overall PhC performance. We demonstrate that, more so than uniform cavity filling, the key to the best filled PhC performance is the precise cavity period and radius values and thickness of the top hafnia layer.

## 1. Introduction

Thermophotovoltaic (TPV) systems are promising as small scale, portable generators to power small robotic platforms, sensors, and portable computational and communication equipment. In TPV systems, thermal radiation from an emitter at high temperature is converted to electricity by a low bandgap photovoltaic (PV) cell. A key factor for the system efficiency is the ratio of in-band emissivity—convertible by the PV cell—relative to the total emissivity. One approach to improve the conversion efficiency is to use two-dimensional (2D) tantalum (Ta) photonic crystals (PhCs) to spectrally tailor the thermal radiation to the PV cell bandgap. Indeed, using this approach we demonstrated a 4.3% fuel-to-electricity system efficiency [1] using PhCs coated with 20–40 nm hafnia as passivation layer.

In theory, dielectric-filled PhCs are a further improvement to coated PhCs. Filled PhCs have high in-band emissivity at a wide range of angles [2], as shown in Figure 1a. Because most thermal radiation is off normal, an omnidirectional filled PhC would increase total in-band radiated power by 55% at 1200 °C [3] compared to an unfilled PhC. Like the coated PhC, a hafnia-filled PhC would also have high-temperature stability and resistance to chemical contamination.





**Figure 1.** Filled PhCs are promising for enhancing thermal emission at all angles, but are difficult to fabricate. a) The optimal filled PhC for cutoff wavelength  $1.8 \mu\text{m}$ , whose structure is shown in the inset, has high in-band emissivity independent of angle. b) Geometric imperfections in the fabricated PhC may explain the shape of the measured emittance spectrum.

However, filled PhCs are difficult to fabricate, largely because the cavity period  $a$  and radius  $r$  are reduced by approximately half (compared to the coated PhC) due to hafnia's high index of refraction ( $\sim 2$ ). The smaller sizes impact the fabrication in several ways: reduced cavity depths  $d$  (due to slower etch rates), more difficult cavity filling (due to higher cavity aspect ratios), and higher sensitivity to slight variations in PhC dimensions. The fabrication process is similar to that described previously [3]. We use atomic layer deposition (ALD) to fill the cavities.

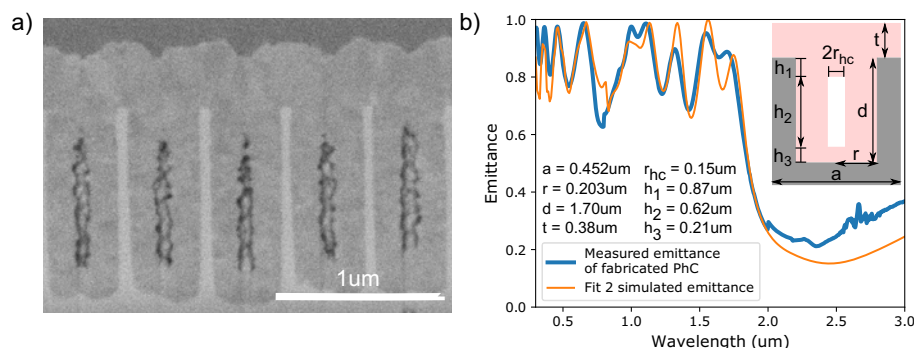
The difficulty of fabrication is reflected in the mismatch between the measured emittance of our fabricated filled PhC and the simulated emittance, as shown in Figure 1b. In our fabricated PhC we have deliberately chosen a shallower depth of about  $1.5 \mu\text{m}$  (aspect ratio  $\sim 4$ ) in order to make the cavity easier to fill.

In this paper we use a combination of focused ion beam (FIB) imaging and simulations to quantify the impacts of fabrication imperfections and provide recommendations for improvement.

## 2. Simulation of Geometric Imperfections

The FIB image (Figure 2a) shows that the cavity filling is incomplete and there is a thick layer of hafnia covering the cavity.

Based on this, we construct a geometric model whose main features are a hollow core and



**Figure 2.** A focused ion beam (FIB) image of the fabricated PhC cavity cross section provides the basis for the geometric model for the fit. a) The FIB image clearly indicates incomplete filling of the cavity and a thick layer of hafnia above the cavity. b) Fit simulation with geometry shown in the inset has a close correspondence with the measured emittance.

thick top hafnia layer. We approximate the hollow core as a cylinder centered at the cavity center, and the hafnia layer as a simple slab (Figure 2b inset). We neglect secondary geometric effects such as scalloping of the top surface and the precise shape of the hollow core.

Our model is sufficient to capture the major features in the measured emittance spectrum: the position of the resonance peaks, cutoff, and shape of the long wavelength emittance, as shown in Figure 2b. The dimensions from the fit are reasonably close to those measured from the FIB. According to our fit, the volume of hollow core is about 21% that of the cavity. Also, the period  $a$  is about 40 nm shorter than that of the optimal PhC. Deviations of the fit from the measured emittance may be attributed to secondary effects such as scalloping of the hafnia layer, variations in cavity size across the sample, and assumptions about hafnia optical parameters.

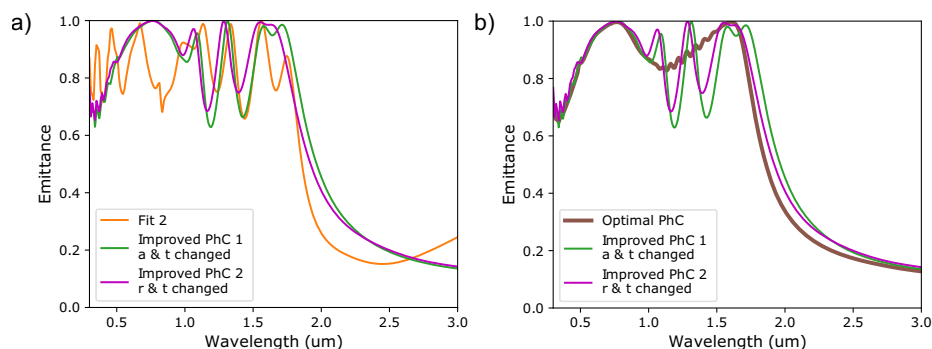
### 3. Recommendations for improvement

Using the structure from the fit as a basis, we investigate what geometrical parameters can be changed to improve the emittance. For our simulations (not depicted) we vary a single parameter at a time while keeping all else equal. For our figure of merit (FOM), we calculate the ratio of the in band power to total radiated power [4], normalized to that of the optimal PhC, at 1200 °C.

However, we find that changing a single variable does not improve the emittance. In particular, increasing the cavity depth makes no difference. Reducing the thickness  $t$  of the top hafnia layer

**Table 1.** Dimensions (in  $\mu\text{m}$ ) of simulated PhCs and their figures of merit (FOM) calculated at 1200 °C for  $\lambda_{\text{cutoff}} = 1.8 \mu\text{m}$ . Bold indicates parameters changed from the fit.

PhC	$a$	$r$	$d$	$t$	Hollow core?	$r_{hc}$	$h_1$	$h_2$	$h_3$	FOM
Optimal	0.49	0.19	3.62	0.063	No	-	-	-	-	1
Fit	0.45	0.20	1.7	0.38	Yes	0.15	0.87	0.62	0.21	0.823
Increased $d$	0.45	0.20	<b>3.62</b>	0.38	Yes	0.15	0.87	0.62	0.21	0.823
Reduced $t$	0.45	0.20	1.7	<b>0.063</b>	Yes	0.15	0.87	0.62	0.21	0.821
No hollow core	0.45	0.20	1.7	0.38	<b>No</b>	-	-	-	-	0.756
Improved 1	<b>0.5</b>	0.20	1.7	<b>0.063</b>	Yes	0.15	0.87	0.62	0.21	0.897
Improved 2	0.452	<b>0.19</b>	1.7	<b>0.063</b>	Yes	0.15	0.87	0.62	0.21	0.905



**Figure 3.** To improve the emittance, it is important to match the optimal  $a$ ,  $r$ , and  $t$  values (see Table 1). a) Compared to the fit, Improved PhCs 1 and 2 show a higher in-band emissivity in the  $\lambda=0.5\text{--}1 \mu\text{m}$  and  $\lambda=1.5\text{--}1.7 \mu\text{m}$  ranges. b) Overall the emittances of Improved PhCs 1 and 2 are close that of the optimal PhC.

to 63 nm increases the in-band emissivity from 0.5 to 1  $\mu\text{m}$  but shifts the cutoff towards a longer wavelength, which effectively increases the out-of-band emissivity. In addition, eliminating the hollow core appears to worsen our emittance according to our FOM (see Table 1).

Instead, it is simultaneously changing both  $t$  and either  $a$  or  $r$  that improves the emittance. As shown in Table 1, we change  $t$  to the optimal  $t$ , and either  $a$  to 0.5  $\mu\text{m}$  or  $r$  to the optimal  $r$ . Compared to Fit 2 (see Figure 3a), both improved PhCs have improved in-band emissivity from 0.3 to 1.0  $\mu\text{m}$  and 1.5  $\mu\text{m}$  to the cutoff. The out-of-band emissivity from the cutoff to 2.7  $\mu\text{m}$  becomes higher but improves from 2.7 to 3.0  $\mu\text{m}$ .

The thickness  $t$  impacts the emittance both above and below the cutoff wavelength. Above the cutoff, the top layer creates Fabry-Perot resonances, whose peak locations can be estimated by considering reflection. Tuning  $t$  to roughly below  $\lambda_{\text{cutoff}}/(4n)$  prevents destructive interference of reflected waves near  $\lambda_{\text{cutoff}}$  and eliminates high emittance above the cutoff. Below the cutoff, the higher emittance is likely due to the hybridization of Fabry-Perot modes and cavity resonances.

As Figure 3b shows, these emittances of the improved PhC actually better match that of the optimal PhC. This suggests that fabricating the correct  $a$ ,  $r$ , and  $t$  to within  $\pm 10$  nm can make a PhC robust against a hollow core. The depth  $d$  appears to be less crucial than  $a$ ,  $r$ , or  $t$ .

#### 4. Conclusions and Future Work

We have found that the mismatch between the measured and the ideal emittance is due to the presence of a hollow core, a thick hafnia layer ( $t$ ), and the deviation of  $a$  from the optimal  $a$ .

However, to improve the emittance it is more important to precisely fabricate the cavity period  $a$  and radius  $r$ , and to reduce the thickness  $t$  of the hafnia layer than to prevent the formation of the hollow core. With new and improved techniques for better geometrical control, such as stepper-based lithography and argon sputtering, it will be possible to achieve  $\sim 90\%$  of the spectral selectivity of the optimal filled PhC.

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