

# Polyatomic Refractory Metastructure for Perfect Absorption and Efficient Thermal Management

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## ABSTRACT

Refractory materials, known for their exceptional thermal stability and robustness in extreme high-temperature conditions, have gained attention in recent years. These materials, including high-melting-point metals, such as titanium, tungsten, chromium, molybdenum, and tantalum, are ideal for applications demanding high-temperature resistance and durability. Here, we present the design of polyatomic refractory metastructures capable of achieving perfect absorptivity as well as near-unity emissivity. We design arrays of clustered refractory-metal nanodisks (tungsten and titanium) coupled to a same-metal backplane with dielectric spacers between the nanodisks and the backplane. Similarly, the spacer is made of refractory materials, silicon nitride and titania, respectively. By tuning the thickness of this spacer, our polyatomic metastructures achieve near-perfect absorptivity and near-unity emissivity across visible and near-infrared spectral ranges (0.4–2  $\mu\text{m}$ ). This work highlights the potential of refractory materials for high-performance absorbers and thermal emitters that are capable of withstanding extreme temperatures without compromising performance, thus paving the way for advancements in energy applications and high-temperature sensing.

**Keywords:** Thermal emitters, metasurfaces, metasystems, metadevices, optical antennas, nanoantennas, perfect absorbers

## 1. INTRODUCTION

Refractory materials have gained considerable attention in recent years due to their exceptional thermal stability and robustness under extremely high-temperature conditions.<sup>1–3</sup> These materials include ceramics and high-melting-point metals and are particularly suited for applications demanding high-temperature resistance and durability. Some of these applications include thermo-photovoltaics, solar energy harvesting, and high-temperature sensing. Refractory materials are essential in thermal management and thermal emitters because they can withstand high temperatures while minimizing heat loss and maximizing efficiency. Effective manipulation of emissivity can be achieved using metastructures through controlled non-local resonances and antenna design, providing promising opportunities for advances in thermal engineering.<sup>4</sup> The necessity for refractory materials is paramount for applications where it is essential to treat the surface of an object with coatings that maintain consistent radiance despite temperature fluctuations, effectively counteracting changes caused by the blackbody emission of the object.<sup>5</sup>

Perfect absorbers are engineered structures designed to absorb nearly all incident electromagnetic waves over a specific wavelength range. The design principle usually involves creating a resonant structure that can trap and dissipate electromagnetic waves efficiently. When these perfect absorbers are made of refractory materials, they can maintain their performance in harsh environments, thereby making them invaluable for efficient energy applications. The foundational work on perfect absorbers has reported on achieving near-unity absorption using metamaterials.<sup>6</sup> Recently, refractory plasmonic materials possessing a high melting point, such as titanium, tungsten, chromium, molybdenum, and tantalum, have been used to create metastructures that exhibit perfect

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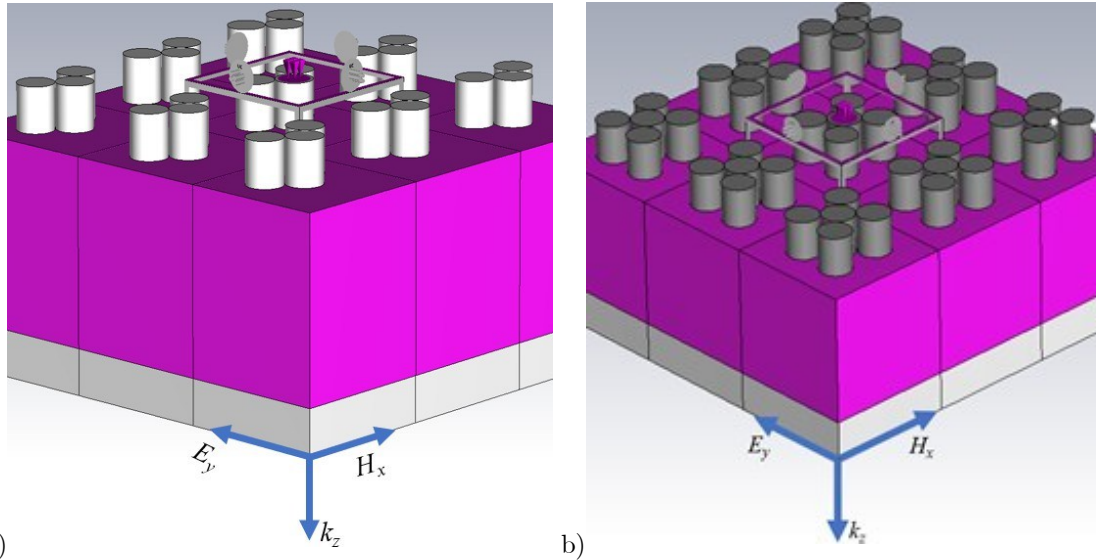


Figure 1. A schematic of the proposed optically thin metastructure consisting of an array of clustered nanodisks: a) three and b) five nanoscaters in the polyatomic unit cell. Nanodisks are made of tungsten or titanium; they have a height of  $H = 60$  nm and a radius of  $R = 25$  nm. The unit cell has a period  $P = 200$  nm in both  $x$ - and  $y$ -directions. The thickness of the spacer (made of silicon nitride or titania) varies from 5 to 250 nm. The metal backplane is assumed to be infinitely thick.

absorption in various wavelength ranges. These metastructures take advantage of the strong and versatile capabilities of their metadesigns in light concentration and localization. They have been utilized in numerous designs as part of absorbers and emitters to strengthen thermal stability and for high performance.<sup>7-10</sup> Refractory ceramics, such as hafnium dioxide, and refractory carbides, such as silicon carbide, offer additional benefits, including chemical inertness and structural stability. These properties make them ideal for use in environments exposed to corrosive agents or mechanical stress.

In this work, we present an engineered polyatomic design of a refractory metastructure capable of achieving perfect absorptivity and near-unity emissivity. We employ arrays of clustered nanodisks (single, three, and five) coupled to a metal backplane substrate. The dielectric spacer is placed between the nanodisks and the backplane substrate, and its thickness is tuned (Figure 1). Our metastructure achieves perfect absorptivity or near-unity emissivity across visible and near-infrared spectral ranges of  $0.4\text{--}2\text{ }\mu\text{m}$ . The near-unity absorptivity of a material implies near-unity emissivity, in accordance with Kirchhoff's law of thermal radiation, which states that for a body in thermal equilibrium, the emissivity is equal to its absorptivity at a given wavelength and temperature, ensuring efficient thermal radiation and energy exchange. We employ tungsten and titanium as refractory metals because of their high melting points and silicon nitride and titania as refractory dielectric in the spacer. Consequently, absorbers made from these materials can withstand extremely high temperatures or harsh environments without any adverse effect on their performance.

## 2. RESULTS

To demonstrate near-unity absorptivity and emissivity in the optically thin metastructure, we select designs consisting of arrays with nanoscaters clusters (polyatomic, Figure 1), as well as a single nanoscaters (monoatomic). Nanodisks are 60 nm tall and have a radius of 25 nm. These nanodisks are placed on top of a dielectric spacer, which is, in turn, positioned on a metal film. The period  $P$  of the design structures is chosen to be 200 nm. The optical properties of our design structures are numerically simulated under normal illumination with a plane wave source polarized in the  $y$ -direction (electric field  $E$  along the  $y$ -axis), implementing the simulations using full-wave numerical simulations in the CST Studio Suite software package. We impose periodic boundary conditions in the  $x$ - and  $y$ -directions and perfectly-matched-layer boundary conditions in the  $z$ -direction.

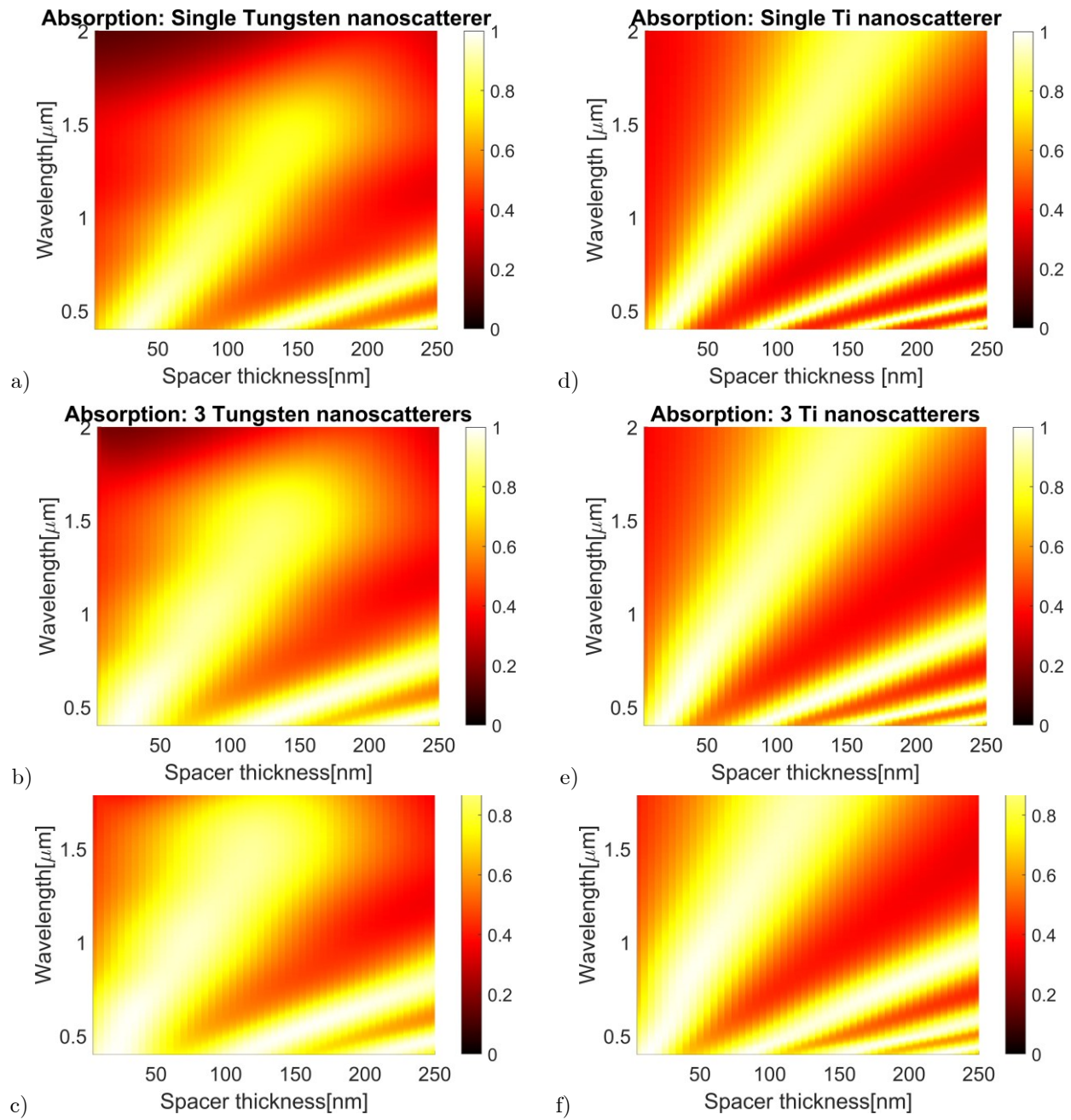


Figure 2. The absorptance in arrays of nanodisks (nanoscatterers) of different combinations: a,d Single nanoscatterer; b,e Three nanoscatterers; and c,f Five nanoscatterers. a,b,c Tungsten and d,e,f Titanium. The metastructures have varying spacer thicknesses.

Nanoantennas can precisely control light scattering by manipulating their geometrical parameters, such as size, shape, and arrangement, which determine the resonance conditions and scattering efficiency.<sup>11–16</sup> Additionally, nanoantennas enable the localization of light at the nanoscale by creating strong near-field enhancements, achieved through plasmonic or dielectric resonances, allowing for concentrated electromagnetic fields in sub-wavelength regions.

The absorptivity spectra for various thicknesses of the spacers for each of the design structures are shown in Figures 2. Tungsten and titanium are metals used for nanodisks and backplanes that operate over a broad wavelength range (0.4–2  $\mu\text{m}$ ). The absorptivity achieves near-unity in dual or triple bands in visible and near-infrared spectra, depending on the spacer thickness. The tungsten nanodisks, in particular, achieve near-unity or perfect absorptivity with a spacer thickness of approximately 125 nm in the visible and near-infrared ranges and 200 nm in the two visible bands, respectively. Similarly, the titanium nanodisks attain near-unity or perfect absorptivity with spacer thicknesses of around 150 nm in the two visible and one near-infrared bands. Additional bands are observed for the case of titanium.

When the performance of two sets of materials is compared, the absorptivity intensity in each of the three designs (five, three, and a single nanodisk) is similar. The primary difference is that, as the number of nanodisks increases, the width of the absorptivity band also increases. The increase in the absorptivity bands is attributed to the fact that as the number of nanodisks increases, it enhances the optical coupling and collective interactions among the nanodisks. As the number of nanodisks increases, the distance between them decreases, leading to stronger near-field interactions. The interactions thus broaden the resonance modes, thereby increasing the overall absorptivity bands. Our results demonstrate the effectiveness of using refractory materials, specifically tungsten and titanium nanodisks, to achieve perfect absorptivity and near-unit emissivity in optically thin metastructures over a broad wavelength range. The choice of tungsten and titanium is driven by their high melting points and excellent thermal stability, which are essential for applications in high-temperature environments. Our simulations reveal that the designed metastructures with varying thicknesses can achieve optimal absorptivity properties.

Polyatomic refractory metastructures can be engineered to develop advanced thermal emitters with highly controlled emissivity profiles, enabling precise thermal management in high-temperature environments. By leveraging the unique optical properties of these metastructures, it is possible to enhance the efficiency and performance of thermal emitters for applications in energy harvesting and infrared sensing. The polyatomic refractory metastructures we report here, characterized by near-perfect absorption, can be utilized for emitters with high emissivity because of Kirchhoff's law, which states that a good absorber is also a good emitter at thermal equilibrium. This principle allows these metastructures to achieve efficient thermal emission, making them ideal for high-performance thermal-emitter applications.

### 3. CONCLUSION

In conclusion, our study presents a comprehensive analysis of optically thin perfectly absorbing polyatomic metastructures using refractory materials. By employing tungsten and titanium nanodisks coupled to a metal backplane substrate with a dielectric spacer, we have demonstrated the capability of these metastructures to achieve perfect absorptivity and emissivity across visible and near-infrared ranges. Effective thermal management using metastructures can be achieved by employing polyatomic nanoantennas to control light scattering. Our findings pave the way for future research and development in high-performance absorbers, which can potentially lead to significant advances in energy applications and high-temperature sensing.

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## REFERENCES

- [1] Li, W., Guler, U., Kinsey, N., Naik, G. V., Boltasseva, A., Guan, J., Shalaev, V. M., and Kildishev, A. V., “Plasmonics: Refractory plasmonics with titanium nitride: Broadband metamaterial absorber,” *Advanced Materials* **26**(47), 7921–7921 (2014).
- [2] Fan, S. and Li, W., “Photonics and thermodynamics concepts in radiative cooling,” *Nature Photonics* **16**(3), 182–190 (2022).
- [3] Wang, B.-X., Xu, C., Duan, G., Xu, W., and Pi, F., “Review of broadband metamaterial absorbers: from principles, design strategies, and tunable properties to functional applications,” *Advanced Functional Materials* **33**(14), 2213818 (2023).
- [4] Islam, M. S. and et al., “Lattice mie resonances and emissivity enhancement in mid-infrared iron pyrite metasurfaces,” *Optics Express* **31**, 40380–40392 (Nov 2023).
- [5] Babicheva, V., Kim, H., and Pique, A., “Temperature-independent thermal radiation using phase-change materials,” (2024).
- [6] Landy, N. I., Sajuyigbe, S., Mock, J. J., Smith, D. R., and Padilla, W. J., “Perfect metamaterial absorber,” *Phys. Rev. Lett.* **100**, 207402 (May 2008).
- [7] Zheng, Y., Yi, Z., Liu, L., Wu, X., Liu, H., Li, G., Zeng, L., Li, H., and Wu, P., “Numerical simulation of efficient solar absorbers and thermal emitters based on multilayer nanodisk arrays,” *Applied Thermal Engineering* **230**, 120841 (2023).
- [8] Zhou, F., Qin, F., Yi, Z., Yao, W., Liu, Z., Wu, X., and Wu, P., “Ultra-wideband and wide-angle perfect solar energy absorber based on ti nanorings surface plasmon resonance,” *Physical Chemistry Chemical Physics* **23**(31), 17041–17048 (2021).
- [9] Zhou, L., Tan, Y., Ji, D., Zhu, B., Zhang, P., Xu, J., Gan, Q., Yu, Z., and Zhu, J., “Self-assembly of highly efficient, broadband plasmonic absorbers for solar steam generation,” *Science Advances* **2**(4), e1501227 (2016).
- [10] Zhou, Y., Qin, Z., Liang, Z., Meng, D., Xu, H., Smith, D. R., and Liu, Y., “Ultra-broadband metamaterial absorbers from long to very long infrared regime,” *Light: Science & Applications* **10**(1), 138 (2021).
- [11] Karimi, V. and et al., “Optical chirality in mxene nanoantenna arrays,” *MRS Advances* **9**, 557–564 (2024).
- [12] Han, A. and et al., “Applicability of multipole decomposition to plasmonic- and dielectric-lattice resonances,” *The Journal of Chemical Physics* **156**, 114104 (03 2022).
- [13] Bosomtwi, D. and et al., “Lattice effect for enhanced hot-electron generation in nanoelectrodes,” *Opt. Mater. Express* **11**, 3232–3244 (Sep 2021).
- [14] Han, A. and et al., “Second harmonic generation in metasurfaces with multipole resonant coupling,” *Nanophotonics* **9**(11), 3545–3556 (2020).
- [15] Babicheva, V. E. and Moloney, J. V., “Lattice zenneck modes on subwavelength antennas,” *Laser & Photonics Reviews* **13**(2), 1800267 (2019).
- [16] Zhukovsky, S. V. and et al., “Giant photogalvanic effect in noncentrosymmetric plasmonic nanoparticles,” *Phys. Rev. X* **4**, 031038 (Sep 2014).