

Efficient computation of thermal radiation from biperiodic layered metasurfaces using the T -matrix method

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(Received 24 August 2025; revised 13 February 2026; accepted 6 April 2026; published 22 May 2026)

Metasurfaces are becoming important tools for the control of thermal radiation. Understanding their functional possibilities on computational grounds requires evaluating the response of the biperiodic layered system for many degrees of freedom, including several radiation directions and polarizations, while varying lattice spacing, thicknesses, and/or materials of homogeneous layers, over a range of frequencies. The diverse set of cases that need to be considered in simulations prompts for efficient numerical tools to handle them. To respond to this need, we present a method for computing the thermal radiation from metasurfaces that combines the directional Kirchhoff's law with efficient T -matrix-based calculations. We show that such a method can accurately reproduce experimental data from a metasurface made of platinum square plates. Additionally, we predict highly circularly polarized emissivity from a chiral metasurface. When comparing CPU-times, the method outperforms other approaches such as rigorous coupled wave analysis already at the modest number of 61 cases per frequency.

DOI: [10.1103/xwt4-mf93](https://doi.org/10.1103/xwt4-mf93)

I. INTRODUCTION

The recent developments in nanotechnology have enabled many new possibilities for constructing two-dimensional periodic arrays of nanoparticles, known as metasurfaces, which enable a refined control of electromagnetic fields. In particular, the design and fabrication of metasurfaces for the control of thermal radiation is an active area of research [1–7], with timely applications such as thermophotovoltaic devices and radiative cooling [8–10]. Numerical methods are used to predict and optimize the desired properties of the metasurfaces [11–13] before their fabrication and experimental characterization.

A key trade-off in these numerical methods is between accuracy and computational cost. While being computationally costly, finite-element methods (FEMs) have become a standard for retrieving reliable reference data because of their high accuracy [14]. On the other hand, other methods such as the rigorous coupled wave analysis (RCWA), also known as the Fourier modal method [15], are applied for their faster computation time while remaining reasonably accurate in suitable planar systems [16].

This work introduces a method for computing angle- and polarization-resolved thermal emission spectra of metasurfaces. It uses a set of precomputed T -matrices, also known as transition matrices [17], and the publicly available TREAMS software library [18] for constructing metasurfaces and computing their optical properties. The metasurfaces are described

in the S -matrix formalism [19], in which the transmittance, the reflectance, and subsequently the absorptivity are calculated. The thermal spectra are then computed using the directional Kirchhoff's law of thermal emission [20], together with the Planck law and the common assumption that the thermal emission of an object at temperature T is independent of its environment [21, §2]. In this work, the T -matrices have been computed using the FEM. We show that the proposed method is able to reproduce experimental data [3] and make predictions about more exotic metasurfaces that have not yet been fabricated. Furthermore, the proposed method can compete with more established approaches such as pure FEM or RCWA in terms of computational costs. Once the T -matrix has been obtained, all frequency-independent computations can be performed within TREAMS in a small fraction of the time that the other solvers require. Therefore, computing optical properties via the T -matrix is an alternative to pure FEMs or RCWA and allows for efficient computation of angle- and polarization-resolved spectra, because a single T -matrix contains all optical properties for a given frequency. A homogenization procedure via quantities like the surface impedance or surface susceptibility [22,23] would lose any information about the granularity of the metasurface. Furthermore, such homogenization procedures are limited to descriptions of systems from subwavelength scatterers [22–24]. The T -matrix method is not subject to such a restriction as it considers multipolar orders larger than the dipolar order and does not assume any limitation on the size of the scatterers or lattice constant relative to the wavelength, enabling simulations of diffracting systems.

For scatterers with a size on the order of micrometers, as in the systems considered in this work, the T -matrices are obtained using methods that solve the Maxwell equations. These methods can be generic such as FEM, finite-difference

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time-domain, or boundary-element methods [25], or specific for particular geometries [26,27]. The T -matrix, however, is a rather generic model and can also be obtained for much smaller objects, such as molecules, using quantum-chemical methods [28,29]. This allows one to compute the thermal radiation of BINOL molecules [30], for example. Therefore, the method presented here can be applied beyond arrays of microparticles, to less common systems containing layers of molecular crystals [31], or graphene patches [2].

We estimate that the method will outperform even RCWA for most metasurfaces. Importantly, the number of cases per frequency, and hence the computational advantage of the proposed method will quickly increase as more degrees of freedom are exploited when optimizing the design. By ‘cases’, we denote all combinations of degrees of freedom of the metasurface that do not change the meta-atoms of which the metasurface is composed. Examples of such degrees of freedom are the lattice kind, lattice spacing, and the material and thickness of homogeneous layers embedding the lattice.

At this point, it is worth mentioning a current limitation of the T -matrix method, namely, the difficulties that arise when computing the interactions between two objects that penetrate each other’s smallest circumscribed spheres. This would affect planar periodic metasurfaces made from tall and thin objects located very close to each other. This issue is under investigation, and there are some proposed solutions [32–38].

The rest of the article is organized as follows. Section II outlines the theory and methods used in the implementation. In Sec. III, the method is applied to a metasurface of platinum particles, and shown to satisfactorily reproduce experimental measurements [3]. Further validation of the method is provided by comparison with RCWA simulations. The computational costs are discussed, including a third option using a full FEM code. Section IV contains the analysis of the thermal emissivity of a chiral metasurface, which consists of a square lattice of copies of a silver helix which was optimized for maximizing its electromagnetic chirality (em-chirality) [39] at a particular frequency. The chiral metasurface features two frequency regions that simultaneously show significant emissivity and a large degree of circular polarization, each region being dominated by a different handedness. Finally, Sec. V concludes the article.

We foresee that the presented combination between the popular T -matrix formalism [40–43], and the efficient treatment of lattices in TREAMS will become a valuable tool for the design of metasurfaces for applications in thermal photonics.

II. THEORY AND METHODS

First, to describe the optical response of an isolated scatterer of a metasurface, we made use of the T -matrix formalism that relates incident and scattered fields by a linear operator, the T -matrix. This operator fully describes the linear light-matter interaction between light and a given object. The T -matrix is typically expressed in the basis of multipolar fields [17]. There are different methods for computing T -matrices, for example the extended boundary condition method [44], the FEM [45], and the discrete dipole approximation method [27].

To compute the thermal radiation from a given metasurface, the emissivity $\mathcal{E}(\hat{r}, \tau, \nu)$ in some direction $\hat{r}$ is determined from the absorptivity $\mathcal{A}(\hat{r}, \tau, \nu)$, according to Kirchhoff’s law of thermal radiation [20],

$$\mathcal{A}(\hat{r}, \tau, \nu) = \mathcal{E}(-\hat{r}, \tau, \nu). \quad (1)$$

The emissivity denotes the ratio of radiation intensity emitted by the metasurface to the radiation intensity that would be emitted by a black body at the same temperature T , at frequency ν with polarization $\tau = \pm 1$, in direction $\hat{r}$. In spherical coordinates, the transformation $\hat{r} \rightarrow -\hat{r}$ to the opposite direction is equivalent to $(\theta, \varphi) \rightarrow (\pi - \theta, \varphi + \pi)$. The meaning of the polarization index τ depends on which polarization basis (circular or s/p) is chosen. In the simulations, we neglect explicit temperature dependence of the material properties. Therefore, Eq. (1) is independent of T . This typically causes some deviations between theory and experiment [8]. The resulting radiance at a given temperature, which can be measured in experiments, can thus be computed by weighing the emissivity by the Planckian radiance spectrum R at the corresponding temperature, which can be expressed depending on the spectral variable as

$$R_\nu(\nu) = \frac{2h\nu^3/c^2}{e^{\frac{h\nu}{k_B T}} - 1} \quad \text{or} \quad R_{\bar{\nu}}(\bar{\nu}) = \frac{2h\bar{\nu}^3 c^2}{e^{\frac{hc\bar{\nu}}{k_B T}} - 1}, \quad (2)$$

where $\bar{\nu}$ denotes wave number, defined as the inverse of the wavelength. The constants h , c , and k_B denote the Planck constant, the speed of light, and the Boltzmann constant, respectively. Kirchhoff’s law of thermal radiation only holds (necessarily) true for reciprocal objects, however, the statement can be generalized [46,47].

A. Computation of the T -matrices

The T -matrices were computed using the FEM solver JCMsuite (JCM) [48] for a range of frequencies. To this end, the three-dimensional meshes of the objects in question were constructed with an edge length at most as long as one fifth of the smallest considered wavelength in the exterior domain, and one fiftieth near sharp edges. Furthermore, the mesh had at least three vertices along each edge of the object. The object was surrounded by a computational domain of a homogeneous, isotropic and lossless material, along with perfectly matched layer boundaries on all sides to mimic an open surrounding. The response of the object to a set of incident multipolar fields was computed and subsequently expanded in outgoing vector spherical harmonics using the built-in MultipoleExpansion method [49]. The expansion coefficients correspond to the T -matrix entries. The number of incident multipolar fields and the expansion order of the outgoing fields (multipolar order) had to be chosen sufficiently large such that all relevant electromagnetic features could be encoded in the T -matrix. More details can be found in the Supplemental Material [50]. The T -matrices resulting from iterating this approach over the selected wavelength range were stored together with metadata in the HDF5 data format [51] and are available via the T -matrix portal.

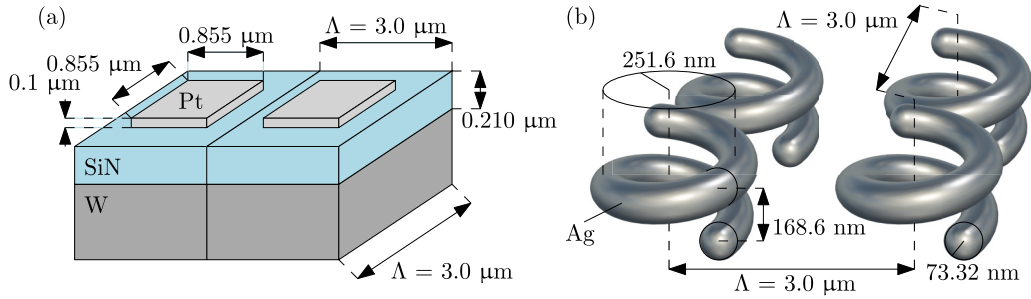


FIG. 1. (a) Schematic perspective view of the square lattice of platinum square plates, with materials and lengths indicated. (b) Four unit cells of a square lattice of silver helices, exemplifying the considered chiral metasurface.

B. Computation of metasurface emissivity

The python library TREAMS was used to compute optical properties of a metasurface constructed from precomputed T -matrices [18]. These T -matrices were converted to PhysicsArray objects and incorporated in a two-dimensional lattice, yielding an effective T -matrix constructed from the cluster T -matrix that represents the entire unit cell, allowing for multiple scatterers per unit cell. The effective T -matrix of a unit cell in the lattice describes the interaction with all other unit cells [52] and is used to obtain the S -matrix, which encodes the response of the metasurface to plane wave illuminations. This procedure involves lattice sums [53] and a change of basis from the spherical to plane waves. The number of plane waves included in this basis has been limited based on their momentum component $k_{\parallel}$, parallel to the metasurface, to those contained in a spherical region in reciprocal space by the factor $b_{\max}$, given by $k_{\parallel} \leq \frac{2\pi b_{\max}}{\Lambda}$. Here, Λ denotes the largest of the lattice constants. This essentially limits the diffraction orders (including evanescent waves) taken into account. The parameter $b_{\max}$ should be chosen as large as possible to include as much of the information from the T -matrix in the resulting S -matrix. However, there is an upper bound to $b_{\max}$, depending on the multipolar order of the T -matrix. Exceeding this limit causes divergent behavior (see Supplemental Material [50]), like shown in the work by Egel *et al.* [54], where the authors analyzed the plane wave expansion of outgoing fields.

The S -matrix of the lattice, together with S -matrices representing other layers of a given metasurface, were combined to construct a single S -matrix representing the entire metasurface. S -matrices representing homogeneous layers, such as substrates, were constructed directly in TREAMS. From the combined S -matrix, the transmittance $\mathcal{T}$ and reflectance $\mathcal{R}$ upon plane wave illumination with frequency ν , at polar angle θ , azimuthal angle φ , and given polarization τ , were directly computed from the corresponding S -matrix entries. The reflectance(transmittance) denotes the perpendicularly outgoing energy flux in the opposite(same) direction of the incident illumination, relative to the incident energy flux. The incident energy flux is given by the time average Poynting vector $\langle S_z \rangle$, where $S_z = \frac{1}{2} \text{Re}(\vec{E}^* \times \vec{H}) \cdot \hat{z}$. The reflected and transmitted energy flux includes all scattered nonevanescent diffraction orders. Explicit expressions for the computation of the transmittance and reflectance coefficients are given in the Supplemental Material of the work by Beutel *et al.* [55]. The directional, polarization, and frequency dependent

absorptivity was consequently obtained as

$$\mathcal{A}(\theta, \varphi, \tau, \nu) = 1 - \mathcal{R}(\theta, \varphi, \tau, \nu) - \mathcal{T}(\theta, \varphi, \tau, \nu). \quad (3)$$

The emissivity was computed using Eqs. (1) and (3).

The thermal emissivities of two different metasurfaces, depicted schematically in Fig. 1, were computed with the methods described above. Section III discusses computations on the square lattice of platinum square plates on a silicon nitride spacer layer and a tungsten substrate, which has been analyzed in experiments by Costantini *et al.* [3], to evaluate whether the methods yield physically accurate results. Simulations with the RCWA method were also performed for additional reference. A second metasurface that has yet to be realized in an experiment was considered for evaluating the thermal radiation of a chiral system with the proposed method. The results are presented in Sec. IV.

III. SQUARE LATTICE OF PLATINUM SQUARE PLATES

The T -matrices of a platinum rectangular cuboid of 0.1 μm in height and 0.855 μm in length and width, surrounded by vacuum, were computed up to multipolar order 10 using the method described in Sec. II A for 121 frequencies linearly spaced in the interval from 45.3 THz to 143.2 THz (1512 cm^{-1} to 4776 cm^{-1}). The permittivity of platinum at these frequencies was taken from the Drude-Lorentz model computations by Rakić *et al.* [56]. By interpolating the T -matrix entries with a piecewise third-order polynomial, the number of T -matrices was increased to 247 evenly spaced T -matrices across this frequency range.

The effective T -matrix was computed in the parity basis for a square lattice with a lattice constant of 3.0 μm and converted to an S -matrix with the choice $b_{\max} = 3\sqrt{2}$. This S -matrix, along with the S -matrices of the homogeneous layers of the stratified system as shown in Fig. 1 were used to compute the absorption coefficients for each wavelength of the interpolated T -matrices, for 35 polar angles from 0° to 70° and azimuthal angles of 0 , $\frac{\pi}{8}$, and $\frac{\pi}{4}$, for both s and p polarizations. The permittivity of the tungsten substrate was taken from Drude-Lorentz model computations by Rakić *et al.* [56], while the 0.210- μm -thick silicon nitride spacer layer was taken to be nonabsorptive with a refractive index of 1.77, like in the work by Costantini *et al.* [3]. This set of S -matrices was stacked together to a single S -matrix [19].

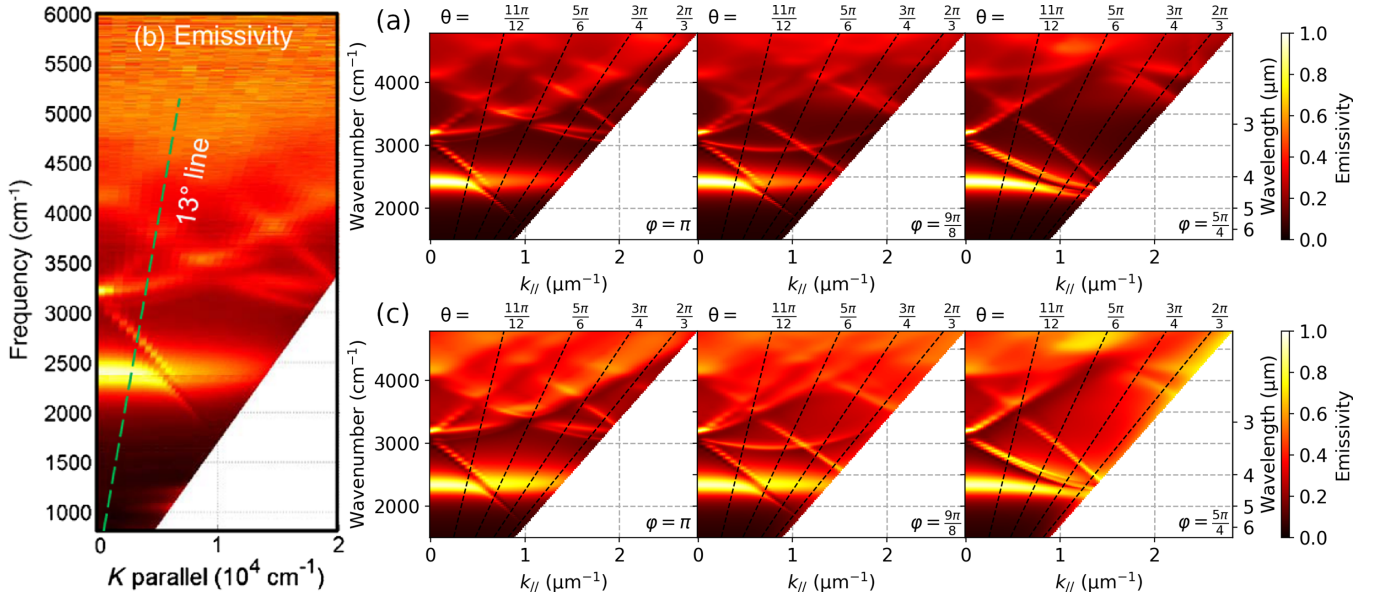


FIG. 2. (a) Polarization averaged emissivities of the platinum square plate metasurface for azimuthal angles $\varphi \in \{\pi, \frac{9\pi}{8}, \frac{5\pi}{4}\}$, computed using TREAMS with T -matrices computed using JCM. (b) Measured polarization averaged emissivity data, at $\varphi = \pi$. Reprinted figure with permissions from Costantini *et al.* [3]. (c) Polarization averaged emissivities of the platinum square plate metasurface computed using the RCWA method, for reference (see Sec. IIIB).

A. Results and discussion

The emissivity spectra from the computations on the platinum square plate metasurface are shown in Fig. 2. The angles of incidence have been converted to momentum components parallel to the surface, according to $k_{||} = k_0 \sin(\theta)$, in order to compare the results to those in the work by Costantini *et al.* [3].

Both simulation results at azimuthal angle $\varphi = \pi$ show the same features as measured in the experiment. Most notable is the relatively broad emissivity feature with a maximum located just below 2500 cm⁻¹. Its position and full width at half maximum can be found in Table I, together with the relative radiance and the radiative efficiency in the “useful window”. The useful window has been defined as a 120 cm⁻¹ wide spectral region around the emissivity maximum, with an opening angle of 13° ($\Omega = 0.84$ sr) [3]. The relative radiance is the emitted power in the useful window compared to a black body in the same window. The radiative efficiency is the emitted power in the useful window compared to the total emitted power of a black body.

From Table I, it is evident that the emissivity peak positions obtained by simulation match the experimentally measured peak position rather well. The RCWA simulations deviate a bit

more compared to the TREAMS simulation, which is due to the convergence behavior of the RCWA (see Supplemental Material [50]). All simulation methods underestimate the width of the peak. This can partly be explained by the fact that the permittivities used in simulation are valid at 298 K, whereas the measurement took place at an elevated temperature of 873 K. The integrated quantities over the useful window are also reproduced quite well. The radiative efficiency of the metasurface being larger compared to that of the black body shows that the thermally radiated power of this metasurface is concentrated stronger in the useful window compared to a black body, which is desirable for applications. Figure 2 also contains predicted emissivities for angles that were not measured, which show significant changes regarding the number and the width of emission lines.

The agreement between our proposed approach, the experimental results, and the RCWA simulations is a valuable validation of our methods and computer codes.

B. Computational costs

Reference spectra using RCWA were computed to compare the accuracy and computational costs of the implementation of the T -matrix method in TREAMS to an established method

TABLE I. Properties of the metasurface emissivity distribution, with measurement data and reported RCWA simulation taken from Costantini *et al.* [3].

	Peak position (cm⁻¹)	FWHM (cm⁻¹)	Relative radiance in ‘useful window’	Radiative efficiency
Measurement	2390	370	85%	3.1%
Reported RCWA	2350	250	—	—
TREAMS	2400	225	84.9%	4.7%
RCWA	2334	305	84.2%	2.9%
Black body	—	—	100%	0.5%

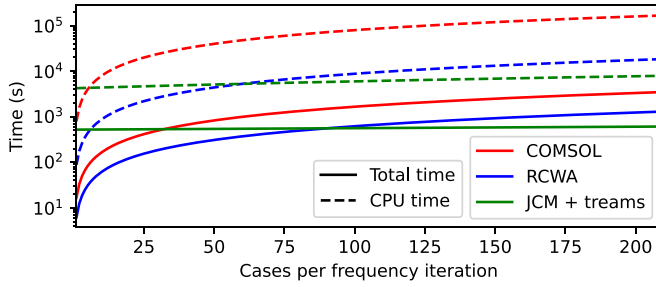


FIG. 3. Computational costs per frequency iteration, as a function of the number of cases sampling the polar angle, azimuthal angle, and polarization at each frequency. All methods scale approximately linearly with the number of cases, with FEM and RCWA having a much steeper slope than the TREAMS simulation, which has a large initial offset due to the fixed computation time of the T -matrix. After about 61 cases per frequency, JCM + TREAMS outperforms the other two methods in CPU-time. Fluctuations in the computation times are not visible on the logarithmic scale.

in computational photonics. RCWA was also used in the work by Costantini *et al.* [3]. The RCWA reference spectra were computed using the FMMA library [57]. The structured layers were represented by a binary mask to model the permittivity contrast. The Fourier series coefficients were computed using this mask and the permittivities of the object and its surrounding material. The fields were computed via the ‘pol’-method described in Liu and Fan [58], with applied damping of strong high frequency Fourier components. This ensured that the fields tangential to the metasurface could be determined with greater accuracy around permittivity transitions.

For further reference, a FEM simulation in the COMSOL software was performed at a fixed angle of incidence to compare the computational costs for a single wavelength.

All simulations were performed on the same hardware, featuring a 2×AMD EPYC 7453 processor, to enable a comparison between the computational costs of these methods. Total computation times (wall-clock time) and CPU-times, which reflect the speedup from multiprocessing, were tracked.

The costs of these computations can be appreciated in Fig. 3 and Table II. The method we propose has a fixed cost per frequency for computing the T -matrices through the FEM simulation. After such cost has been paid, TREAMS is comparatively very fast in sampling different incident angles and polarizations, but also layer thicknesses, lattice spacings, and unit cell arrangements, for each frequency. We denote one specific set of these parameters as ‘case’ per frequency. The computational time of TREAMS increases linearly with the number of cases, but with a slope that is much smaller than those of RCWA or FEM. This can be seen in Table II where

TABLE II. Average computational cost for different methods, per frequency iteration, per case.

Method	CPU-time (s)	Total time (s)
FEM (COMSOL)	1.9×10^2	39
RCWA	75	5.3
TREAMS	0.42	0.42

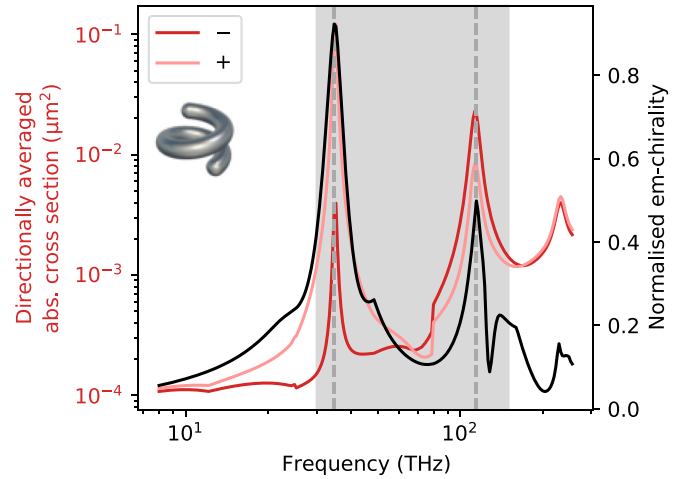


FIG. 4. Frequency dependence of the helicity-dependent absorption cross section of a single silver helix, optimized for maximizing its em-chirality. Different helicities are denoted by different shades of red, together with the frequency dependence of the normalized em-chirality of a single silver helix in black. The gray shaded region indicates the frequency range used for lattice computations. The frequencies of the absorption maxima are indicated by the dashed vertical lines.

the computation times per frequency per case for different methods are listed. Accordingly, Fig. 3 shows crossings of the computational costs of JCM + TREAMS with the other two methods, as the number of cases per frequency increases.

We highlight that such crossings are modest numbers of cases per frequency, that are likely to be insufficient for the characterization of thermal radiation, in particular when working with very asymmetric metasurfaces [6] or systems that radiate in very narrow angular ranges [1]. Additionally, using RCWA is rather awkward for some geometries, such as the helices investigated in the next section. Importantly, the number of cases per frequency, and hence the computational advantage of the proposed method, will quickly increase as more degrees of freedom are exploited for optimizing the design, such as the lattice kind, lattice spacing, the material and the thickness of homogeneous layers embedding the lattice.

The memory used by the different methods was 14, ~2.4, 19, and 1 GB for any particular frequency iteration, for COMSOL, RCWA, JCM, and TREAMS, respectively.

IV. CHIRAL METASURFACE

The chiral metasurface consisted of a square lattice of metallic silver helices in vacuum. The parameters of the single helix were a radius of $r_h = 251.6$ nm and a wire radius of $r_w = 73.32$ nm with 1.407 right-handed turns at a pitch of $p = 168.6$ nm. The ends of the helix wire were rounded off by spherical caps. These parameters were taken from a silver helix optimized for a large em-chirality [39], adjusting for different ambient material parameters. The optimization procedure was similar to the one by Garcia-Santiago *et al.* [59]. Selected properties of the isolated single helix are shown in Fig. 4. This figure shows that the single helix has a strong chiral absorption around 34.8 THz, where the em-chirality

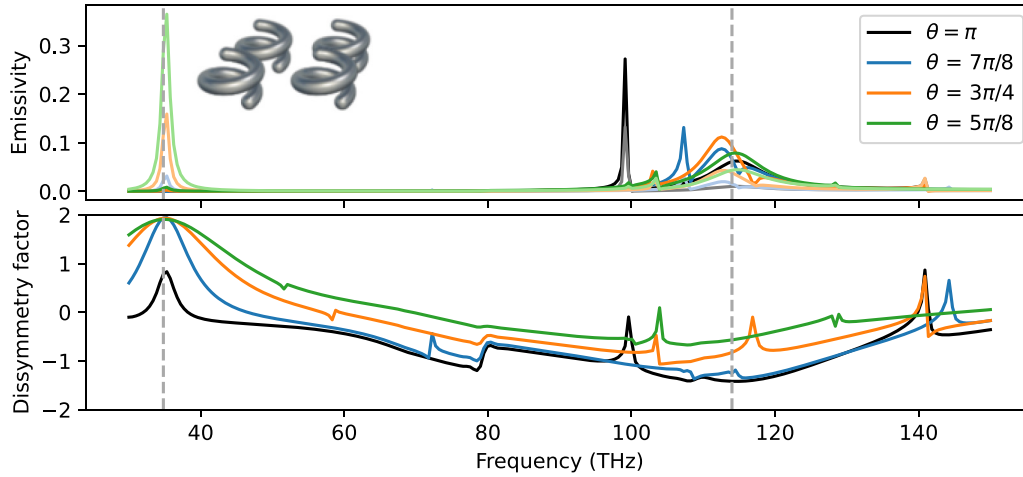


FIG. 5. Helicity-dependent emissivity of light from the two-dimensional array of silver helices and dissymmetry factor for different polar angles, in the frequency range marked by the shaded region from Fig. 4. Right-handed and left-handed circular polarizations are indicated by solid and pale colors, respectively.

reaches 92.3% of its upper bound. An em-chirality of 100% would correspond to an object that is invisible to one of the two helicities. Notably, the right-handed helix interacts predominantly with positive helicity (left-handed circularly polarized) light at the strong chiral absorption. Another absorption peak is located at 114 THz, favored by light with negative helicity (right-handed circular polarization), albeit with a smaller difference in the absorption between the two helicities, resulting in a lower em-chirality. The T -matrices of the helices contained five multipolar orders and were passivated over the considered frequency range by imposing positive semidefiniteness of the imaginary unit times the skew-Hermitian part of the corresponding reactance matrix [60]. This corresponds to setting the optical gain to zero. This was necessary because of numerical noise in the T -matrix from the more complicated geometry and the relatively small size of the helix compared to the wavelength. As described above, the effective T -matrix of the lattice was computed using TREAMS and converted to an S -matrix. The lattice constant was set to $3 \mu\text{m}$ and the number of diffraction orders was limited by $b_{\text{max}} = 3$. The reflection and transmission coefficients of the lattice were computed for four polar angles from π to 0 , for both left- and right-handed circular polarizations. The emissivity was computed from the absorptivity. To analyze the circular polarized light, the computations were in this case performed in the helicity basis.

A. Results and discussion

To compare the emissivity of left- and right-handed circular polarized light, the normalized emissivity difference, also referred to as the ‘thermal g factor’,

$$g_{\text{th}} = 2 \frac{\mathcal{E}_+ - \mathcal{E}_-}{\mathcal{E}_+ + \mathcal{E}_-}, \quad (4)$$

was computed. The emissivities $\mathcal{E}_{\pm}$ together with g_{th} are shown in Fig. 5. This figure shows that the emissivity peaks in frequency regions where the single helix has a large absorption cross section in Fig. 4. At 35.3 THz, g_{th} reaches

its maximum of almost 2, resulting in almost helicity-pure thermal radiation at this frequency. The emissivity maximum corresponding to the 34.8 THz absorption cross section peak is slightly blueshifted, while the emissivity maximum corresponding to the 114 THz absorption cross section peak is redshifted compared to the single helix. It is remarkable that the emissivity, in combination with the large dissymmetry factor, results in thermal radiation with strongly favored and opposite helicity at these frequencies.

Because of the chosen lattice spacing of $3 \mu\text{m}$, the spectrum also shows several lattice resonance peaks, depending on the angle of incidence, at which the emissivity is increased noticeably compared to nearby frequencies. The dissymmetry factor is also affected by the lattice resonances, showing deviations from the otherwise smooth behavior. The lattice resonance with the smallest transverse momentum, corresponding to normal incidence, lies at 99.9 THz. For incidence at an angle, the lattice resonances are weaker and lie at lower frequencies. The feature around 80 THz in the dissymmetry factor plot is due to a numerical artefact from concatenating two sets of T -matrices to a single frequency range.

Overall, emissivity of negative helicity light is stronger at large frequencies, while the emissivity of positive helicity light is stronger at smaller frequencies, as can be seen in the bottom row of Fig. 5.

V. CONCLUSION AND OUTLOOK

In this work, we analyzed thermal radiation from meta-surfaces by using a T -matrix-based method in combination with the directional Kirchhoff’s law. We showed that the implementation of the T -matrix method in TREAMS, with T -matrices computed using a FEM solver, is able to reproduce experimental measurements. The more critical points of the method are the computation of the T -matrix, which has to be of sufficient multipolar order to achieve accurate results, and the convergence of the lattice sums, which requires one to limit the momentum transfer in lattice interactions. The method is expected to be inadequate when the objects in

the planar lattice invade each other's smallest circumscribing sphere.

The method is more efficient than established methods based on RCWA or FEM as soon as the number of cases per frequency exceeds some threshold. For a given metasurface, the number of cases is the total number of radiation directions and polarizations for which the emissivity is computed. Beyond that threshold, the fixed cost of computing the T -matrices already pays off, since for a fixed frequency, each case only requires a computation in TREAMS, which is comparatively very fast. For the metasurface measured in [3], the threshold was 61 cases for RCWA and 6 cases for FEM. We expect that the threshold would be exceeded for most metasurfaces. Moreover, the optimization of metasurfaces for the control of thermal radiation may require to evaluate different kinds of lattices, a range of lattice constants and/or variations of the thickness and material of homogeneous layers. Exploiting these degrees of freedom will significantly increase the number of cases, making the implementation in TREAMS a useful and competitive tool for designing metasurfaces for thermal photonics, for example using an inverse design approach [61–63] or via machine learning [64]. We foresee future developments in this field, not least because of applications to the computation of thermal radiation properties. The method could also be applied to metasurfaces whose

unit cells are made of atomic clusters, such as molecular crystals or arrays of graphene patches, for example. For such cases, the T -matrix can be obtained using quantum-chemical methods.

ACKNOWLEDGMENTS

I.F.-C. and C.R. acknowledge support by the Helmholtz Association via the Helmholtz program “Materials Systems Engineering” (MSE). L.R. acknowledges support by the Karlsruhe School of Optics & Photonics (KSOP). L.R., I.F.-C., and C.R. acknowledge support by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 258734477 – SFB 1173. M.N. and C.R. acknowledge support by the KIT through the “Virtual Materials Design” (VIRTMAT) project. The authors are grateful to the company JCMwave for their free provision of the FEM Maxwell solver JCMSuite.

DATA AVAILABILITY

The data that support the findings of this article are openly available via the DAPHONA portal [65]. The code used for numerical simulations is publicly accessible [70].

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