Design of a Frequency Selective Structure With Inhomogeneous Substrates as a Thermophotovoltaic Filter

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Abstract-In this paper, the design of a thermophotovoltaic (TPV) filter with high-pass characteristics is presented. The filter is in the form of a frequency selective structure (FSS) with cascaded inhomogeneous dielectric substrates. The goal is to allow for more design flexibility using dielectric periodic structures to deliver a sharper filter response. Therefore, the primary focus is to design a periodic material substrate composition (supporting FSS elements) using a topology optimization technique known as the density method. The design problem is formulated as a general nonlinear optimization problem and sequential linear programming is used to solve the optimization problem with the sensitivity analysis based on the adjoint variable method for complex variables. A key aspect of the proposed design method is the integration of optimization tools with a fast simulator based on the finite element-boundary integral method. The capability of the design method is demonstrated by designing the material distribution for a TPV filter subject to pre-specified bandwidth and compactness criteria.

Index Terms—Frequency selective structures (FSS), material design, optimization, thermophotovoltaics (TPVs), topology.

I. INTRODUCTION

F REQUENCY selective structures (FSS) find widespread applications as filters in microwaves and optics [1], [2]. An application relates to thermophotovoltaic (TPV) cell panels [3], which are used in the production of small lightweight portable generators, hybrid electric vehicles and electric grid independent appliances. A need exists to protect the TPV panels from broadband radiation by employing high efficiency spectral control filters. However, these filters often lack compactness, good high-pass behavior or desired efficiency. Here, we present the design of such a TPV filter with high-pass characteristics in the form of a FSS with cascaded inhomogeneous dielectric substrates. The goal is to allow for more design flexibility using dielectric periodic structures to deliver a sharper filter response.

Although the basic operating principles and analysis techniques of FSS structures are well known and studied extensively

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in the past [4]–[6], their vast suite of applications has engendered only few design techniques, almost all heuristic or experimental in nature [7]–[10]. Moreover, design has primarily focused on FSS shape and on the selection of uniform dielectric layers. There are very few design examples, in which the material attribute is explored directly as a design variable [11], [12]. Our primary focus in this study is to design a periodic material substrate composition (supporting FSS elements) using a topology optimization technique known as the density method [13]. More specifically, the density method is extended to develop full three-dimensional substrate designs for a TPV filter. Since typical electromagnetic problems often require several constraints and numerous variables/design cells, a theoretically well-founded mathematical programming algorithm is necessary. The sequential linear programming (SLP) [14] method is such an algorithm and is adopted here for optimization. The evaluation of the response (transmissivity) sensitivity with respect to changes in the design variables (dielectric permittivities) is an essential aspect of any optimization scheme. Here, the adjoint variable method [15] is employed for that purpose to enable versatility and fast convergence using first order mathematical programming algorithms. This paper presents the topology design methodology capable of generating novel configurations through the integration of design optimization tools with robust finite element-boundary integral (FE-BI) simulators [16]. The latter removes limitations on geometry or material distribution but most importantly it incorporates fast O(N) solvers for a rapid solution of large-scale problems.

The aim of the presented design study may be summarized as follows: 1) Explore the possibility of improving spectral filter response via a volumetric material design; 2) Design a spectral filter to be used in a TPV cell with specific design requirements; and 3) Demonstrate the capability of the density method to design for the topology and material distribution of high frequency EM scattering devices. In the following, first the TPV concept and design requirements are introduced. This is followed by a description of the formal design optimization technique to determine the volumetric material distribution. The density method is then extended to design the material distribution for a TPV filter subject to pre-specified bandwidth and compactness criteria.

II. DESIGN SPECIFICATIONS

Thermophotovoltaics is the conversion of secondary thermal radiation, re-emitted by an absorber or heat source into electricity by a semiconductor device. The device is designed for

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Fig. 1. Illustration of the TPV concept.



Material

TABLE I Available Substrate Material for TPV Filter

Material	ε _r
Calcium Fluoride (CaF)	1.96
Barium Fluoride (BaF ₂)	1.35
Yttrium Aluminum Garnet (YAG)	3.6
Zinc Sulfide (ZnS)	4.84
Zinc Selenide (ZnSe)	5.76
Silicon (Si)	11.56
Gallium Arsenide (GaAs)	11.56
Indium Phosphide (InP)	10.89

Fig. 2. Illustration of the ideal filter transmissivity.

maximum efficiency at the wavelength of the secondary radiation. Therefore, its efficiency can be improved by imposing a spectrally selective filter between the heat source and the TPV cell. A schematic illustration of the TPV concept is shown in Fig. 1. Potential applications are: cogeneration, space power source and remote/portable power source.

Our goal is to design an efficient TPV spectral-control filter that complies with specific operational characteristics. Its working wavelength band is 1 μ m–10 μ m and the primary functional requirement is to provide recuperation of low energy photons for the emissive power of the photon radiator. Assuming zero absorption, this translates into a filter design that experiences a sharp transition in its transmissivity characteristics at 2.4 μ m, the onset of inter-band absorption in the TPV device. Ideally, the filter is desired to reflect 100% of the received energy above 2.4 μ m and be totally transmissive below 2.4 μ m. The required ideal response is displayed in Fig. 2. However, in practice, these figures of merit are around 90% and 10%, respectively, due to unavoidable inherent system losses.

Among the expected performance requirements is the filter's insensitivity to angle of incidences and polarization. In addition, a compact structure is desired with a manufacturing limitation on the minimum possible surface dimension of 0.1 μ m. The available material list for dielectric substrates is given in Table I [17]. It is noted that these materials are actually lossy but are assumed lossless here since our goal is to demonstrate the design methodology.

III. DESIGN METHOD

To satisfy the design requirements for the spectral filter, a two-step design procedure is adopted. First, a preliminary design approach is pursued by cascading the FSS with homogeneous dielectric layers. The aim is to determine the FSS shape and initial substrate configuration for the filter. The second step is to improve the filter response using the proposed automated design approach and determine the optimum material distribution. This is discussed in the next section.

A. Topology Optimization Via the Density Method

Simply stated, design via topology optimization implies the determination of the best arrangement given a limited volume of available (electromagnetic) material within a spatial domain subject to delivering optimal (electromagnetic) performance of the concept design. The optimization process systematically and iteratively eliminates and re-distributes material throughout the domain to obtain a concept structure. Unlike other design approaches involving size and shape optimization, topology optimization methods have the advantage of representing arbitrary topologies without re-meshing or complex shape functions. The design method proposed here is based on the density method also known as the solid isotropic material with penalization (SIMP) method. This method has been accepted as a potential design tool in the mechanical engineering area for more than a decade because of its simplicity and efficiency. It allows the synthesis of a device starting from any arbitrary topology. A key aspect of the design method is that any device, not known a priori, is represented by specifying the material properties at every point of the fixed design domain. In practice, to specify the material properties, the design space is discretized into material cells/finite elements. This is the essence of the design method in which the material grating is achieved by introducing only a single density variable, ρ , and relating it to the actual

material property of each finite element through a continuous functional relationship. This density variable, ρ , is related to the material property (the relative permittivity ε_r) and can be physically interpreted as the density of the material whose properties are proportional to ρ^n . A suitable density function, for the dielectric permittivity would be

$$\rho = \left[(\varepsilon_{\rm int} - \varepsilon_{\rm air}) / (\varepsilon_{\rm orig} - \varepsilon_{\rm air}) \right]^{1/n} \tag{1}$$

where n is a penalization factor whereas ε_{int} and $\varepsilon_{\text{orig}}$ are the intermediate and original solid material permittivities, respectively. The factor n is introduced to penalize the intermediate value of the density function. Similar to the standard on/off representation of geometries, the problem is formulated through the introduction of a normalized density with $\rho = 0$ corresponding to a void/off ($\varepsilon_{\text{int}} = \varepsilon_{\text{air}}$), $\rho = 1$ to solid/on ($\varepsilon_{\text{int}} = \varepsilon_{\text{orig}}$) and $0 < \rho < 1$ to a graded intermediate dielectric material, ε_{int} . This parameterization casts the problem in a general nonlinear optimization framework. More specifically, the normalized density within each finite element is used as the design variable to formulate the topology/material optimization problem.

The goal in the density method is to arrive at the optimum distribution of material (densities) such that a desired performance merit of a device is optimized subject to certain design constraints. This is achieved by assigning different density values from 0 to 1 in each design cell to represent the material variation from cell to cell. Unlike conventional design methods, such as the boundary variation or on/off representation of the design domain, the density method arrives at the optimum topology by distributing the material in the form of a gray scale image and updating it using common gradient based mathematical programming techniques. The density design method is then used in conjunction with standard optimization algorithms to achieve optimal material distribution designs for dielectric substrates such as those used in constructing high-pass frequency selective volumes.

The iterative optimization scheme chosen here, due to its well-known efficiency and reliability is the SLP method, employing the DSPLP package in the SLATEC library [18]. SLP is chosen here because it is robust, efficient and easy to use. Moreover, it has been successfully used in similar large-scale topology optimization problems [19]. The essence of the SLP routine is to replace the objective function and constraints by their linear approximations at each iteration. Updates of the design variables are carried out via a procedure based on the adjoint variable method, an efficient method that permits full interface with the FE-BI electromagnetic solver. The adjoint variable method is advantageous because it relies on exact sensitivities which are easily computed. Only one additional analysis run is required versus two or more for other approximations such as finite differences used for derivative calculations. As a result, three-dimensional large scale design problems are formulated and solved efficiently. The sensitivity analysis corresponds to the evaluation of the response (transmissivity) changes with respect to the design variables (dielectric permittivities). For our design problem, the objective is a mathematical function in terms of the transmissivity $|\tau|$ at each frequency. As expected, the objective function depends on the unknown variables. For our case, it is more specifically given by $|\tau| = f(E(\varepsilon), \varepsilon)$, where ε refers to the element dielectric permittivity, which is the parameter to be optimized. This real function $|\tau|$ is differentiated with respect to the complex variable E, the electric field, by following the steps discussed in more detail in [20].

The sensitivity analysis is crucial to integrating the solver with the SLP optimizer. Application of hybrid methods such as the FE-BI to infinite periodic structures provides for a full 3-D modeling flexibility and allows for designing arbitrary geometrical and material details. By virtue of the finite-element method and its O(N) memory and CPU requirements, this module is an ideal candidate for practical FSS analysis without limitations on shape and topology, or substrate material distribution. Accurate results have already been obtained for scattering and radiation applications demonstrating the method's capability [21], [22] including noncommensurate structures [23].

The ultimate algorithm for the proposed design cycle consists of the following iterative steps: 1) Simulation of the device performance using the FE-BI solver with pre-specified data; 2) Solution of the adjoint system equations of the original problem for the sensitivity analysis; 3) Optimization of the volumetric material distribution of the dielectric substrate using an SLP algorithm; and 4) Update of the design variables (densities/permittivities) relying on the interpolation scheme of the density function. Convergence is achieved when changes in the objective function value drops below a certain value (on the order of 10^{-3}).

IV. DESIGN OF THE TPV FILTER

A. Preliminary Design of a High-Pass TPV Filter

When designing a FSS for a specific application, numerous parameters need be considered. Among these are layer specifications, array lattice factor, FSS element type and dielectric properties with the periodic element choice being most critical in determining the resonance characteristics of the design. Various element shapes have been considered in the past [4], [5] and may be categorized into the following six groups: wire (dipole combinations) and slot type elements, wire or slot loop elements, aperture type elements, fractal elements, elements constructed from dielectric perforations and combinations of all possible elements.

Based on the high bandwidth requirements, we choose to consider a square aperture FSS as our initial design. Within this class, square apertures are less sensitive to polarization and typically exhibit a broad bandwidth. Therefore, they are attractive to satisfying a broad range of design requirements. Stacked layers of FSS elements may also be included to control the response if necessary.

Following basic design guidelines, primarily based on the FSS resonance behavior, and the well-known quarter-wavelength transformer ($\lambda/4$) characteristics, the preliminary design resulted in the particular configuration shown in Fig. 3 after a number of design iterations. This is a double layer noncommensurate FSS structure with square aperture shapes. Since the edge length of the square aperture in each layer is the same as the periodicity, we will hereon refer to this structure as a



Fig. 3. Illustration of the preliminary spectral filter design with double layer FSS sandwiched between $\varepsilon_r = 3.6$ substrates. Dimensions are in μ m.



Fig. 4. Transmissivity response for preliminary spectral filter design depicted in Fig. 3.

square aperture FSS. The dielectric substrate is chosen to be an amorphous Yttrium Aluminum Garnet with $\varepsilon_r = 3.6$, an intermediate dielectric value among the available materials listed in Table I. This material satisfies the smallest possible dimensions for manufacturing purposes and yet is compact.

Our efforts to improve the roll-off response of the square aperture FSS ended up with the dual layer square aperture FSS of the illustrated design. The lattice/periodicity of this FSS is 0.56 μ m with an overall dielectric thickness of 0.896 μ m. That is, the structure is rather thick as compared to the lattice dimensions. The periodicity of the top FSS (FSS2) is 0.56 μ m and the periodicity of the lower layer FSS (FSS1) 0.504 μ m, i.e., smaller. That is, this is a two layer noncommensurate design. The inner square dimensions for FSS2 and FSS1 are 0.448 μ m and 0.392 μ m, respectively. Both FSSs are sandwiched symmetrically between dielectric layers with the constant dielectric properties assumed lossless. The transmission response (or transmissivity) of the square aperture filter design is depicted in Fig. 4 and is quite attractive in terms of the pre-specified transmission metrics except for the oscillation at around 1.5 μ m wavelength. It is noted however that the modeling of the stacked FSS layers with different periodicities (viz. a noncommensurate FSS structure) suffers from numerical inaccuracies due to inherent approximations in imposing field continuity at the corners of the FSS periodic cells [23]. As a result of this approximation the FSS apertures at the interfaces may appear larger leading to a transmissivity which can be slightly greater than unity. This is the price we had to pay to have an analysis code that also provides the flexibility to design a broadband FSS consisting of multiple FSS layers, each having a different periodicity. Without this approximation in treating the multilayer noncommensurate FSS, it would be impractical to include the FSS analysis code within the design loop. At the same time, the approximation implies that the resulting transmission coefficient can be greater than "unity" at some frequencies. It would have been appropriate that we also carry out the "exact" analysis of the final design to obtain the precise FSS transmissivity response. Unfortunately, we do not have (to our disposal) an exact analysis code for the noncommensurate structure. Nevertheless, the employed analysis code has been validated extensively [24], and our full expectation is that the "exact" analysis will yield the same transmissivity except for the areas where the approximate design exceeds unity. Therefore we proceeded to truncate the transmissivity to unity whenever it exceeded this value at any point. This is obviously apparent in Fig. 4 between 2 μ m and 2.5 μ m, and the same approach will be followed for all future calculations.

Attempts to remove the unwanted oscillations of the resulting filter's response via FSS design employing traditional homogeneous substrates were not successful. We therefore proceeded to explore changes in the dielectric composition of the substrate. This is addressed next.

B. Topology Optimization of Dielectric Material Distribution for the TPV Filter

To pursue the optimization, we begin with a preliminary design composed of cascaded planar periodic square aperture FSSs sandwiched between multiple dielectric blocks/layers as illustrated in Fig. 3. As evident, in the initial configuration, the dielectric layers on which the FSS are printed are of constant composition.

The primary design focus is the desirable high-pass behavior up to 2.4 μ m with a sharp transition in the transmissivity at the band-gap wavelength of 2.4 μ m. Based on this requirement, a general nonlinear optimization problem is formulated as follows:

Minimize
$$\sum_{\lambda_i=1}^{2.4} (|\tau_{\lambda_i} - 1|)^2 + \sum_{\lambda_i=2.4}^{10} (|\tau_{\lambda_i} - 0.1|)^2$$
 (2)

subject to the following constraints:

$$\sum_{1}^{N} \rho_i \cdot V_i \le V_T \cdot \eta \tag{3}$$

$$0 \le \rho_i \le 1.0. \tag{4}$$

Here, (2) represents the objective function with τ_{λ_i} being the transmissivity at wavelength λ_i . A minimization of the square sum of errors for sampled transmissivity values corresponds to the desired high-pass behavior. V_T in (3) is the total volume of the design domain, i.e., the prescribed volume of the periodic unit cell; η is the fraction of the design domain to which the designed material is limited. As defined earlier, ρ_i is the ith density of the ith finite element/pixel that comprises the dielectric volume. We also remark that the constraint (3) provides for a restriction on the maximum design domain. And the other constraint (4) assures that the density variable stays within feasible limits.

A minimum of the objective function corresponds to a performance with a high transmissivity value, i.e., $\tau \sim 1.0$ for wavelengths between 1–2.4 μ m and little transmission, i.e., $\tau \sim 0.1$ is set for wavelengths beyond that range (2.4–10 μ m). Therefore, evenly spaced frequency points are chosen to ensure accurate capturing of the transmissivity response especially at the high frequency spectrum. To avoid high CPU costs for the simulation, only up to 4.6 μ m (65 THz) instead of the entire spectrum were considered since the transmission behavior is not as affected by material variations at higher wavelengths.

The formulation and solution of the optimum material distribution problem complies with the proposed topology optimization procedure. Accordingly, the optimization problem is solved iteratively via the SLP method and the densities are updated at each design iteration via an automated process. As noted earlier, the densities are related to the actual permittivity values of the substrates where ε_{solid} is the chosen material from Table I and $\varepsilon_{air} = 1.0$ (air) with possible penalization factors. To ensure an adequate amount of supporting material within the substrates, the value of η is chosen accordingly to limit the amount of dielectric substrate with $\varepsilon_r = \varepsilon_{solid}$.

The initial design variables and parameters are based on the geometrical attributes of the initial square aperture design depicted in Fig. 3. Normal incidence and transverse electric (TE) polarization are assumed as the excitation. As discussed before, the sensitivity of the objective function with respect to the density variables is derived via the adjoint variable method [15]. It



Fig. 5. Optimization history for spectral filter design with double layer FSS geometry (Fig. 3). Design parameters: n = 2, $\eta = 60\%$, $\varepsilon_{\text{solid}} = 4.84$ (ZiS) and $\varepsilon_{\text{initial}} = 1.1$.



Fig. 6. Transmissivity for initial ($\varepsilon = 1.1$) versus optimized material distribution of the TPV filter with double layer FSS geometry (Fig. 3). Design parameters: n = 2, $\eta = 60\%$, $\varepsilon_{\text{solid}} = 4.84$ (ZnS) and $\varepsilon_{\text{initial}} = 1.1$.

is remarked that the move limits are set at $\Delta x_{\min} = 0.001$ and $\Delta x_{\max} = 0.01$ to ensure stable convergence and these values were chosen from experience.

V. DESIGN RESULTS

Having an initial design with a response close to the desired transmission performance (see Fig. 4), the focus was next to improve the response of the filter via the proposed design procedure described above. The design algorithm is adopted for the same exact optimization model defined in the previous section with an initial homogeneous "air like" dielectric substrate of $\varepsilon = 1.1$ instead of $\varepsilon = 3.6$ to allow for guaranteed feasibility of the volume constraint for "sufficient" amount of solid material ($\eta > 50\%$). The entire volumetric substrate of the FSS was discretized into 16 slabs resulting in a total of 3048 finite elements each with their own individual dielectric constants. The surface mesh details are given in Fig. 3. Specifically, the substrate below FSS1 was discretized into 4 layers along the thickness with a surface mesh comprised of 162 $(9 \times 9 \times 2)$ triangular surface elements. Also, the substrate sandwiched between FSS1 and FSS2 was discretized into 8 layers, with each layer discretization in 200 ($10 \times 10 \times 2$) triangular surface elements. Finally, the dielectric volume above the FSS2 was subdivided



Fig. 7. Optimized material distribution across each layer (counted from bottom) for TPV filter with double layer FSS geometry (Fig. 3) and corresponding density (ρ) color scale (top). Design parameters: n = 2, $\eta = 60\%$, $\varepsilon_{solid} = 4.84$ (ZnS) and $\varepsilon_{initial} = 1.1$.

into 4 layers also with 200 ($10 \times 10 \times 2$) triangular surface elements per layer.

For our design, the penalization factor was set to n = 2 and the volume fraction is set to $\eta = 60\%$. Validity of the simple mixture averaging formula is assured since the dimensions of the structure are much smaller as compared to the resonance wavelengths in the required high-pass region. Consequently, to achieve smooth mathematical convergence and to prevent intermediate material properties in the final design, the volume constraint was necessary. More specifically, sharper topologies with improved performance may be obtained if the volume constraint is active (satisfied as an equality) with the volume fraction yielding an approximate effective dielectric constant of around 3.3. This value corresponds to an average central resonance wavelength of the desired high-pass region. The solid material chosen for the design was zinc sulfide with $\varepsilon_{\rm solid} = 4.84$ (Table I). This would allow for 60% of solid material allocation via the active volume constraint and permit a feasible effective dielectric substrate to retain the required high-pass behavior up to 2.4 μ m. This 60% proportion of

solid material is preferred to simplify the fabrication of the designed filter. With a volume fraction of $\eta = 60\%$ and an initial (air-like) structure ($\varepsilon_{\rm initial} = 1.1$), the resulting effective dielectric constant will be $4.84 * 0.6 + 1.1 * 0.4 \sim 3.3$.

Convergence was achieved in 23 iterations as depicted in Fig. 5. For this case, the design CPU time was 1 hour and 9 minutes on a Pentium 3 Processor (about 3 min/iteration). We observe in Fig. 6 the remarkable improvement achieved in the truncated transmissivity response as compared to the initial performance. Key to achieving this performance was the optimal distribution of the available material within the 16 layers of the design domain (as illustrated by the density distribution in Fig. 7). Fig. 7 is a color image where each grey-scale level corresponds to a value of ε_r .

The actual fabrication of the double layer FSS filter was not pursued but is a major challenge that requires emerging techniques in micro-fabrication. The distorted shapes at the outer edges of the solid (dark) material and the presence of a subtle amount of intermediate material within the light shade pixels (ε is not equal to 1.1 but larger than 1.34) present additional fabrication challenges. Increasing the penalization factor or other techniques could lead to simpler designs for fabrication purposes [12], [25], [26] but are not pursued here. Even though we did not present a verification (viz. measurements) of the design, we should point out that our analysis method and computer code has been validated for FSS with similar dimensions [24]. Moreover, the proposed design dimensions can be realized in practice as recently reported in [27].

VI. CONCLUSIONS AND REMARKS

The design of a spectral filter in the form of a FSS for TPV applications was presented. A two-step design procedure was introduced to achieve a sharp high-pass behavior of a compact, yet efficient filter that would comply with the given design requirements. Using existing design guidelines, we began the formal design process using a double noncommensurate square aperture FSS sandwiched between homogeneous dielectric substrates. This material was subsequently optimized via the density method to obtain the substrate material topology subject to the TPV filter performance. It was shown that significant performance improvements were attained via optimization of the material topology. We do remark, however, that prior to fabrication the obtained gray scale image need be altered via a gradual penalization technique and image processing/filtering approach to achieve a manufacturable solid design. The simplicity and low number of iterations and CPU time needed to reach convergence motivates the application of the proposed design method for other electromagnetic applications.

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