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Robust optimization of a tandem grating solar thermal absorber

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ABSTRACT

Ideal solar thermal absorbers need to have a high value of the spectral absorptance in the broad solar spectrum to utilize the solar radiation effectively. Majority of recent studies about solar thermal absorbers focus on achieving nearly perfect absorption using nanostructures, whose characteristic dimension is smaller than the wavelength of sunlight. However, precise fabrication of such nanostructures is not easy in reality; that is, unavoidable errors always occur to some extent in the dimension of fabricated nanostructures, causing an undesirable deviation of the absorption performance between the designed structure and the actually fabricated one. In order to minimize the variation in the solar absorptance due to the fabrication error, the robust optimization can be performed during the design process. However, the optimization of solar thermal absorber considering all design variables often requires tremendous computational costs to find an optimum combination of design variables with the robustness as well as the high performance. To achieve this goal, we apply the robust optimization using the Kriging method and the genetic algorithm for designing a tandem grating solar absorber. By constructing a surrogate model through the Kriging method, computational cost can be substantially reduced because exact calculation of the performance for every combination of variables is not necessary. Using the surrogate model and the genetic algorithm, we successfully design an effective solar thermal absorber exhibiting a low-level of performance degradation due to the fabrication uncertainty of design variables.

1. Introduction

An ideal solar thermal absorber should have a high absorptance in the broad solar spectrum to maximally convert the solar radiation to heat. With naturally existing materials, broadband absorption is difficult to be achieved because most natural materials absorb the light at specific wavelength due to their intrinsic electronic and atomic structures [1]. Not relying on the materials intrinsic absorption properties, numerous studies have designed a broadband solar thermal absorber by employing various nanostructures, such as metallic gratings [2,3], thin-film multilayers [4–6], photonic crystals [7,8], and nanocomposites [9,10]. Key to achieving broadband absorption by using a periodic array of the nanostructures, whose characteristic dimension is comparable to or smaller than the wavelength of solar radiation, is to superpose multiple electromagnetic resonances, such as surface plasmon polariton, cavity resonance, and magnetic polariton, in a similar wavelength region. Recently, Wang et al. [11] numerically designed the broadband solar absorber by arranging two different sized tungsten square patches on tungsten thin film and SiO_2 thin film. In addition, Chang et al. [12] designed the solar absorber by employing a vertically-aligned tungsten nanowires. However, those studies have limitations in designing absorbers through parametric studies only. In fact, little changes in design variables of complex geometries could change the electromagnetic resonance condition as well as their coupling mechanism, which makes the absorptance of nanostructures harder to be precisely predicted before the actual fabrication. Therefore, the optimization of high-performance solar thermal absorber based on complicated nanostructures are difficult to be achieved soley by parametric studies. On the other hand, there have been research that performed optimization to maximized the performance of nanostructures for applications in thermophotovoltaic emitter [13], low-emissivity glass [14,15], broadband absorber [16], and radiative cooling [17]. However, those studies focused on the performance itself without considering the robustness of performance with respect to unintended variations in design variables.

As mentioned earlier, a broadband absorber utilizes complicated structures of several tens to hundreds nanometer scale to exploit various electromagnetic resonances and their coupling. Precise fabrication of such nanostructures requires tremendous efforts in time and cost, and there always exists unavoidable fabrication uncertainties in conventional MEMS processes [18,19]. Random variations in design variables due to fabrication errors affect the

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resonance phenomena, which in turn results in different (usually deteriorate) performance compared to the design value. By employing the robust optimization, any variation of intended performance can be taken into account during the design process and thus can be minimized.

In this work, the robust optimization is performed to minimize the undesirable absorptance variation due to the fabrication error for a tandem grating solar absorber previously proposed by Han et al. [20]. The robust optimization is one of optimization methods searching for the performance which is not largely affected by uncertainties or variation in input variables. Critical design variables affecting the performance of the absorber will be selected through parametric study, and 300 random sample points will be constructed through the Latin hypercube method [21]. Solar absorptance corresponding to each sample points will be calculated by employing a finite-difference-time-domain (FDTD) simulation. A surrogate model will be constructed with 300 sets of design variables and solar absorptance data corresponding to each set of design variables via the Kriging method [22]. Using the surrogate model and the genetic algorithm, we will seek an optimum combination of design variables with high absorptance and low variation of the absorptance when the design variables have uncertainty [23].

2. Parametric study of a tandem grating solar absorber

Prior to the robust optimization, parametric study was conducted to investigate the effect of each design variable on the performance of the solar absorber. The structure considered here is a tandem grating solar absorber [20] that consists of a 400-nm-thick tungsten substrate, a silicon dioxide (SiO_2) film, a two-dimensional (2-D) tungsten nanohole array filled with SiO_2, a SiO_2 layer, and a 2-D tungsten nanodisk array. For the parametric study, the period (Λ), the diameter of the tungsten nanohole (D_h) and the nanodisk (D_d), and the thickness of the upper (t_{ou}) and the lower (t_{ob}) SiO_2 film, are selected as design variables, whereas the thicknesses of nanohole (t_h) and nanodisk (t_d) are assumed to be the same as the reference design. Here, the reference design is set to be $\Lambda = 500$ nm, $D_h = 200$ nm, $D_d = 300$ nm, $t_{ou} = t_{ob} = t_h = t_d = 50$ nm, which was initially proposed by Han et al. [20]. For quantitative comparisons, the solar absorptance of the tandem grating solar absorber is calculated in the solar spectrum by

$$\alpha_{sol} = \frac{\int_{300\ \mathrm{nm}}^{2000\ \mathrm{nm}} \alpha_\lambda G_{dsi}(\lambda) d\lambda}{\int_{300\ \mathrm{nm}}^{2000\ \mathrm{nm}} G_{dsi}(\lambda) d\lambda} \tag{1}$$

where α_λ is the spectral absorptance, and $G_{dsi}(\lambda)$ is the direct solar intensity at air mass 1.5. To calculate the spectral absorptance of the tandem grating solar absorber, the FDTD simulation is performed, and the commercial software, Lumerical is employed. In the simulation, plane waves are incident perpendicular to the structure, and a frequency domain power monitor is placed above the plane wave source. Both ends of the z-direction have a perfectly matched layer, and a periodic boundary condition is applied to the x- and y-directions. Mesh is a cube of 2.5 nm in size, and numeric convergence according to the mesh size has been confirmed. The auto shutoff ratio is set to be 10^{-6}. The optical properties of the tungsten and SiO_2 are from the tabulated data [24] embedded in the software. The FDTD simulation took approximately 2 hours in a cluster (4 nodes) with a total of 8 Intel Xeon processors (3.00 GHz) for obtaining an absorptance spectrum.

Fig. 1(a) shows the calculated spectral absorptance according to the change of Λ while other design parameters remain unchanged. For the reference design, the spectral absorptance exhibits multiple peaks at wavelength (in vacuum) $\lambda = 410$ nm, 519 nm, 719 nm and 1795 nm as well as slight enhancement near 1139 nm. First, absorption peaks at 410 nm and 519 nm are due to the Wood's anomaly that can be predicted for normal incidence by [25]

$$\left(\frac{2\pi}{\lambda}\right)^2 = \left(\frac{2\pi i}{\Lambda}\right)^2 + \left(\frac{2\pi j}{\Lambda}\right)^2 \tag{2}$$

where i and j stand for the diffraction order in the x- and y-direction, respectively. The above equation predicts that the Wood's anomaly can be found at $500/\sqrt{2} = 353$ nm when $(i, j) = (1, 1)$ and at 500 nm when $(i, j) = (1, 0)$ or $(0, 1)$. As can also be seen from Fig. 1(a), the absorption peak due to the Wood's anomaly shifts to the lower wavelength region (i.e., blueshifted) as the period becomes smaller, which is completely consistent with Eq. (2).

In Fig. 1(a), the absorption peak at $\lambda = 1139$ nm is broader than others, but the corresponding absorptance value is smaller. In order to identify which electromagnetic resonance mode is responsible for such enhancement, we plot the time-averaged square of the electric field normalized to the incident electric field. As can be seen from Fig. 1(b), a strong electric field is localized around the tungsten nanodisk, suggesting that localized surface plasmon (LSP) is excited at the nanodisk [26]. Notice that LSP associated with the tungsten nanodisk should also be observed when the nanodisk is free standing. Although it is not shown here, we also calculate the reflectance of the free-standing tungsten nanodisk and confirm that the absorption peak $\lambda = 1139$ nm is indeed due to the excitation of LSP. Because the size of the tungsten nanodisk is fixed, the localized surface plasmon hardly changes with the period Λ.

The absorptance peak at $\lambda = 1795$ nm is due to the excitation on the magnetic polariton (MP), as briefly explained in the following. The time-averaged square of the magnetic field normalized to the incident magnetic field is plotted in Fig. 1(c). It can be clearly seen from Fig. 1(c) that anti-parallel currents are induced at both ends of the upper tungsten nanodisk and the lower tungsten nanohole, resulting in a strong magnetic field confined in the sandwiched SiO_2 layer [27]. In order to predict the resonance condition of MP, an equivalent inductor-capacitor (LC)-circuit model [28] is employed. The equivalent LC-circuit model predicts that the fundamental mode of MP occurs at $\lambda = 1734$ nm. As the period Λ decreases, the absorptance peak associated with the MP is redshifted slightly [see Fig. 1(a)], which is also consistent with the equivalent LC-circuit model. This is because the capacitance due to SiO_2 region between the neighboring nanodisks increases as Λ decreases.

Finally, the absorptance peak at $\lambda = 719$ nm is due to the cavity resonance in the SiO_2 region confined by the tungsten nanodisk array, as can be seen from the magnetic field distribution in Fig. 1(d). It is clear that the magnetic field is localized in the SiO_2 area that fills the region outside of the tungsten nanodisk. This localized magnetic field seems like the magnetic polariton, but it is not because tungsten does not behave like a metal at this wavelength. In order to confirm whether it is the cavity resonance mode, we employ the following equation:

$$\frac{\lambda}{n_{SiO_2}} = \frac{2}{\sqrt{\left(\frac{l}{w_x}\right)^2 + \left(\frac{m}{2w_z}\right)^2}} \tag{3}$$

where n_{SiO_2} is the refractive index of SiO_2, w_x and w_z are the horizontal and vertical size of the cavity, respectively, and (l, m) represents non-negative integers [2,29]. If we approximate $w_x = 200$ nm and $w_z = 100$ nm for the reference design, the cavity resonance mode of $(l, m) = (1, 0)$ occurs at $\lambda = 580$ nm, which seems far apart from the absorptance peak at $\lambda = 719$ nm. It should be noted that the above equation is strictly valid for a rectangular cavity and the considered tungsten nanodisk does not provide such a rectangular cavity. In fact, w_x indicates the minimum distance between neighboring nanodisks, and thus, the *effective* size of the cavity in the x-direction could be slightly larger than w_x. For example, if we simply change the horizontal size of the cavity to 250 nm, then