Research article

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Compact disordered magnetic resonators designed by simulated annealing algorithm

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Abstract: Sub wavelength all-dielectric structures processing simultaneously electric and magnetic resonances provide a new horizon for tailoring magnetic light–matter interaction that is often overlooked in optical spectrum. In general, the magnetic field enhancement can be boosted by utilizing the magnetic resonances of dielectric resonators where structural disorder effect is considered as a parasitic negative effect for the targeted response. Here, in contrast, we theoretically propose and experimentally demonstrate that compact disordered dielectric resonators with substantial enhancement of free-space magnetic field can be automatically designed by the combination of simulated annealing algorithm and numerical solution of Maxwell's equations, providing an alternative for tailoring magnetic light–matter interaction. The functionality and reliability of the proposed concept are further verified by microwave experiment. Our results might facilitate the application of compact disordered magnetic resonators in enhancing magnetic dipole transition of quantum emitter, magnetic resonance imaging, wireless power transfer and beyond.

Keywords: disordered all-dielectric resonators; nanophotonics; optical magnetic field enhancement.

1 Introduction

Light–matter interaction mainly relies on the electric component of light because most natural materials have

very weak response to the magnetic component of light [1, 2]. However, such magnetic component of light plays important roles in optical physics, such as the studies of magnetic dipole transition [3–7], sensing [8, 9] and optical magnetic imaging [10]. In general, the enhancement of magnetic field in optical spectrum can be achieved by the surface plasmon effect [11–16], where sophisticated artificial metallic nanostructures, such as butterfly shape [17], gold triabolo shape [18] and spherical shell shape [19], are employed to boost the response of nanostructures to the magnetic component of light. The combination of plasmonic and dielectric structures can even achieve the ideal magnetic dipole scattering in optical spectrum [20]. However, the metallic nature of plasmonic structures inevitably results in giant Ohmic loss during the light–matter interaction. As a result, all-dielectric metamaterials provide effective alternatives for manipulating magnetic resonances with much smaller absorption loss compared with their metallic counterpart [21]. By tailoring the modal properties of an all-dielectric nanostructure, one can realize low loss resonant enhancement of magnetic field in optical spectrum [22–28], which can facilitate the amplification and manipulation of magnetic Purcell effect [29–32]. A conventional mean for further enhancing magnetic light–matter interaction relies on ordered structure such as resonant metasurface or photonic crystals slab [33–39]. In these cases, parasitic disordered effects during the fabrication process are generally considered as negative effects as they will reduce the total Q factor of the resonances.

Recently, the application of artificial intelligence in nanophotonics enables a paradigm shift for the design and optimized mechanisms of electromagnetic device compared with conventional intuition-based approaches [40–53]. For example, evolutionary algorithms might be favored in designing nanophotonic components and devices whose targeted functionalities are featured with completed non-convex objective functions [41–48]. Alternatively, simulated annealing algorithm (SAA) is used to mimic the process of annealing and cooling [54, 55], where the Metropolis rule is applied to facilitate random search of parameters. Compared with the genetic

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algorithm, which is usually influenced by the parent generation and tends to be local optimized for a limited population, SAA is more favorable to obtain the global optimization with a limited computation power. At the same time, SAA would be more applicable for the question where unveiling an approximate global optimum is more important than finding a precise local optimum in a fixed time cost [54, 55].

In this paper, we theoretically propose and experimentally demonstrate a new and automated method to design disordered all-dielectric resonant structures supporting magnetic hot-spots in free space utilizing the combination of SAA and numerical solutions of Maxwell equations. The proposed method is quite general which is validated by several examples under different plane wave excitation scenarios. The working frequency can be scaled according to Maxwell's equations and a proof-of-concept microwave experiment is conducted to verify the numerical results.

2 Results

2.1 The combination of SAA and the solution of Maxwell's equations for designing disordered magnetic resonators

Because the generality of Maxwell's equations in the electromagnetic spectrum, we design the disordered resonant structures in the microwave range first, which will be experimentally validated in the following section. In order to acquire the enhancement factor of magnetic field on a specified surface of the disordered structures under the excitation of a linearly polarized plane wave, we numerically solve Maxwell's equations by finite element method (FEM by HFSS, Ansoft). The SAA is used for coordinating the FEM to search disordered structures with the maximized magnetic field enhancement in a given frequency range. Figure 1(a) and (b) outline the procedure of the combination of SAA with the numerical solution of Maxwell's equations and the schematic of the SAA algorithm which can avoid local optimum, respectively. First of all, we use the SAA and FEM to find an ordered structure (lattice constants D_x and D_y) with the largest magnetic field enhancement on a given surface of the structure in a specified frequency band. Then, it is used as an input of the first iteration of the SAA, whose objective function F_n of the n th iteration corresponding to the largest magnetic field enhancement factor of the disordered structure will be compared in the next iteration,

$$F_n = \max(f_n(\omega_1), f_n(\omega_2) \dots f_n(\omega_m)) \quad (1)$$

where $f_n(\omega_m)$ is the largest enhancement factor of magnetic field amplitude among all spatial points on a plane above the surface of the structure at the frequency ω_m . The objective value $f_n(\omega_m)$ is evaluated in a frequency band consisted of m frequency points. Then, the structure under consideration is searched by disordered perturbation from such an ordered rectangular array (a $N \times N$ array consisted of dielectric cylinders with radius R and height h) with two lattice constants D_x and D_y , as shown in Figure 1(c). The disordered perturbation will be generated by the following rule:

$$s_{n+1} = s_n + T_n * \frac{A}{\text{norm}(A)} \quad (2)$$

$$A = \text{randn}(1, nva)$$

where s_n is a matrix consisted of the random deviations of geometry parameters (i.e., Δx_{lm} and Δy_{lm}). Δx_{lm} and Δy_{lm} are the random deviations of coordinates for the dielectric resonator located at the l th row and the m th column of the array, as shown in Figure 1(c). l and m are integers between 1 and N . T_n is the current temperature annealed for the n th iteration. A is a normal distribution random matrix, where the value of nva is $2N^2$. The following Equation is used to update the coordinate parameters of the disordered resonators during the iteration,

$$\begin{aligned} x_{lm} &= l * D_x + \Delta x_{lm} \\ y_{lm} &= m * D_y + \Delta y_{lm} \end{aligned} \quad (3)$$

Here, x_{lm} and y_{lm} are the coordinates of the resonators in the rectangular array. It should be pointed out that there are in principle infinite realizations of disordered structures, the reason why we consider disordered structures perturbed from periodic structures is because structures with moderate disordered deviation from the ordered structure might benefit from both the collective resonant effects of ordered structure and the field localization leveraged by the small group velocity near the band edge. Therefore, we optimize the disordered structure in a limited perturbation strength $|s_{n+1}| \leq |3R/8|$, which also prevents the disordered resonators from spatial overlapping. If one of the variables in s_{n+1} is out of this region, it will be renewed according to the equation (4):

$$\begin{aligned} s_{n+1} &= \beta * s_{n+1} + (1 - \beta) * s_n \\ \beta &= \text{rand}(0, 1) \end{aligned} \quad (4)$$

Subsequently, the plane wave excitation of the updated disordered structure is calculated by the FEM to evaluate the objective function F_n . The Metropolis rule is used

Figure 1: (a) The procedure of combining simulated annealing algorithm (SAA) with the solution of the Maxwell's equations by the finite element method (FEM). (b) The SAA is a random search algorithm which means that it accepts a solution which is worse than the current solution based on the Metropolis rule, so it is possible to jump out of the local optimum solution, which might facilitate the achievement of the global optimal solution. (c) The SAA is used to determine the ordered structure (D_x and D_y) with the largest magnetic field enhancement on a certain plane above the structure under the excitation of a plane wave. Then, random perturbations Δx_{lm} and Δy_{lm} generated by SAA are coupled back to the FEM to search for the largest magnetic field enhancement (objective function F_n) on that plane.

to determine whether the results will be accepted as the current value of objective function F_n :

$$\begin{cases} 1, & \text{if } F_{n+1} > F_n \text{ \& } p > \text{rand}(0, 1) \\ 0, & \text{if } F_{n+1} \leq F_n \text{ \& } p < \text{rand}(0, 1) \end{cases} \quad (5)$$

where $p = \exp\left(-\frac{F_{n+1}-F_n}{T_n}\right)$ is the probability of accepting a new solution and rand is corresponding to the uniform random distribution. It should be pointed out that we do not reduce the temperature T_n (fixing at 100) of SAA for the results presented in this paper since we would like to maintain a more global search of disordered structures [56]. Compared with the results where the temperature is reduced for every 100 iterations under the condition of $T_{n+100} = 0.95 \tilde{n} T_n$, the optimized disordered resonant structure based on our modified SAA outperforms the conventional one (data not shown here). This is mainly because we would like to obtain a tradeoff between time cost and global optimization under limited computational power [Intel(R) Core(TM) I7-6700 3.4 GHz]. Finally, the optimization process is truncated at the 200th iteration.

2.2 Numerical results

We consider the optimization of disordered resonant structure utilizing the combining of SAA with the solution of Maxwell's equations for two typical cases of plane wave excitation. The first case is shown in Figure 2(a) where a 5×5 rectangular array of all-dielectric resonators is excited by a Z-polarized plane wave propagating along the Y axis.

The radius R and height h of all cylinders are 8 and 11 mm, respectively. The permittivity we used is 9.6 which is corresponding to the alumina ceramic we used in microwave experiment. We neglect the loss of the all-dielectric structure first and a loss tangent of 8×10^{-4} will be included in the simulation in order to compare with experimental results in the following section. The achieved magnetic field enhancement factors at different iterations (denoted as current value) and the best one up to the present iteration (denoted as best value) for all iterations are shown in Figure 2(b). It can be seen from the figure that the current values of objective function F_n are randomly distributed, where some of the current value and the best value are the same at certain iterations. The step jump of best value indicates the combination of SAA and the Maxwell's equations can prevent the solution from local optimums. It can be also seen that the best value become convergent for a sufficient large number of iteration. Figure 2(c) presents the spectra (blue line) of the largest normalized magnetic field $|H_z|$ on the plane 1 mm above the disordered structure where the normalization is referred to the incident plane wave. As can be seen from this figure, the enhancement factor of the disordered structure is almost 30 times larger than that of the incident plane wave at 5.875 GHz. The corresponding result (red line) of the optimized ordered structure (D_x is 26.14 mm and D_y is 26.08 mm) is shown for comparison. Counter-intuitively, the maximized enhancement factors of the disordered structure outperform the ordered one in a broad band manner. The distribution of magnetic field at the optimized condition with imposed disordered structure profile is shown in Figure 2(d) where resonant magnetic hot-spots of free space can be achieved.

Figure 2: (a) The schematic of the all-dielectric disordered resonators. The polarization of the plane wave is marked in the inset. The structure is placed on a substrate with a smaller permittivity. The radius R and height h of all resonators are 8 and 11 mm, respectively. The lattice constants of the ordered 5×5 array are $D_x = 26.14$ mm and $D_y = 26.08$ mm, respectively. (b) The largest enhancement factor of magnetic field $|H_z|$ (best value) and the temporary one (current value) obtained on the plane 1 mm above the structure during the iteration of optimization. (c) The spectra of the largest enhancement factor of magnetic field $|H_z|$ calculated for the disordered and ordered structures, respectively. The largest magnetic field enhancement is achieved at 5.86 GHz for ordered structure and 5.875 GHz for disordered structure. (d) The calculated normalized magnetic field $|H_z|$ distributions of the optimized results

(5.875 GHz) of the disordered structure on a plane 1 mm above the surface of the structure.

We further consider a different excitation scenario indicated in Figure 3(a) where the disordered structure is optimized to enhance magnetic field along the propagation direction of the plane wave. As can be seen from Figure 3(b), the proposed method can indeed avoid local optimum. The largest enhance factor is 7.16 which is smaller than the case shown in Figure 2 since the magnetic field along the propagation direction is indirectly induced by the electromagnetic near-field interaction, as can be

seen from Figure 3(c). The corresponding result (blue line) of the optimized ordered structure ($D_x = 22.76$ mm and $D_y = 25.62$ mm) is shown for comparison. The maximized enhancement factors of the disordered structure also outperform the ordered one in a broad band manner. It should be pointed out that the achievable maximum magnetic field enhancement and the realization of homogenous magnetic field enhancement in a compact structure is a trade-off. These numerical results indicate

Figure 3: (a) The schematic of the all-dielectric disordered resonators. The polarization of the plane wave is marked in the inset. The radius and height of all resonators are the same as Figure 2. The lattice constants of the ordered 5×5 array are $D_x = 22.76$ mm and $D_y = 25.62$ mm, respectively. (b) The largest enhancement factor of magnetic field $|H_z|$ (best value) and the temporary one (current value) obtained on the plane 1 mm above the structure during the iteration of optimization. (c) The spectra of the largest enhancement factor of magnetic field $|H_z|$ calculated for the disordered and ordered structures, respectively. The largest magnetic field enhancement is at 5.92 GHz for ordered structure and 5.935 GHz for disordered structure. (d) The normalized magnetic field $|H_z|$ distributions at the optimized results (5.935 GHz) of the disordered structure on a plane 1 mm above the surface of the structure.

clearly that the compact disordered structure intentionally perturbed from the ordered one resembles an effective mean to boost the magnitude of magnetic field in free space, which could serve as an alternative of the digital case [46]. As the permittivity we use is close to certain semiconductor materials in optical spectrum, it can be scale to the optical spectrum which will be addressed in the following section.

2.3 Experiment results and discussions

In order to validate the numerical results, we perform the experiment similar to the excitation situation of Figure 2(a). The experimental setup is shown in Figure 4(a), where the standard gain horn antenna (HD-58SGAH20N) is connected to a vector network analyzer (VNA, RS-ZNB40) to mimic a linearly polarized plane wave source. The home-make coil antenna is fixed on the microwave scanning platform (Linbo, NFS03 Floor Version) connected to the VNA, where the acquired $|S_{21}|$ is proportional to the magnetic field amplitude $|H_z|$. The disordered structure is composed of alumina ceramic resonators (the permittivity is 9.6) placed on a foam substrate (permittivity is close to 1). The radius and height of the resonators are the same as the case of Figures 2 and 3. Microwave absorbers are placed around the equipment setup to minimize the echo effect.

The distance between the horn antenna and the sample is larger than 10 times of the central working wavelength to minimize the discrepancy between the experimental microwave source and the ideal plane wave, as indicated in Figure 4(a). In order to prevent the probe (radius of the coil is around 1 mm) from touching the sample, the probe is approximately 3 mm away from the upper surface of the sample. We measure the S_{21} on a plane above the sample when the sample is presented first. Then, we remove the sample and measure the same area again under the same excitation condition. Finally, the enhancement factor of magnetic field amplitude is obtained by normalizing the $|S_{21}|$ accordingly. Then the largest field enhancement within the measured area for every frequency considered can be found in one measurement. The experimental results (blue open circles) at 5–6 GHz are shown in Figure 4(b). As we can see from this figures, the experimental results qualitatively agree with the numerical results (red solid line) where the absorption loss of dielectric materials is considered. The largest measured enhancement factor (16.51) is achieved at 5.8675 GHz while the calculated one (16.41) is 5.875 GHz, where the discrepancy between numerical and experimental results might be originated from the imperfect home-make magnetic probe and the imperfect plane wave excitation utilizing the horn antenna. We further provide the distributions of simulated magnetic field (normalized $|H_z|$) and the measured normalized $|S_{21}|$ in

Figure 4: (a) The experimental setup for measuring the near-field enhancement of magnetic field. (b) The measured frequency dependence of enhancement factors of $|S_{21}|$ that is proportional to the magnetic field $|H_z|$ and the corresponding calculated maximum of magnetic field enhancement factor on a plane 3 mm away from the surface of the structure. (c) and (d) The corresponding calculated normalized magnetic field $|H_z|$ and measured $|S_{21}|$ distributions at the maximum of magnetic field enhancement, which are achieved at 5.875 and 5.8675 GHz, respectively. The resolutions of Figure 4(c) and (d) are 0.8 and 2 mm, respectively.

Figure 5: (a) The spectra of the largest enhancement factor of optical magnetic field $|H_z|$ obtained on the plane 10 nm above the structure. The structure under considered is a disorder structure perturbed from a 5×5 array. The radius and height of all resonators are 80 and 110 nm, respectively. The permittivity of the resonator is 9.6. (b) The corresponding normalized magnetic field $|H_z|$ distributions of the optimized result (507.6 nm). The incident plane wave is indicated in the insets. (c) The spectra of the largest enhancement factor of optical magnetic field $|H_z|$ obtained on the plane 10 nm above the structure under the other excitation condition as shown in d). The radius and height of all resonators are the same as Figure 5(a). (d) The corresponding normalized magnetic field $|H_z|$ distributions of the optimized result (508.04 nm). The incident plane waves are indicated in the insets.

the Figure 4(c) and (d), respectively, where a reasonable agreement between two cases is achieved. In general, the fabricated sample contains parasitic disordered effect. According to the experimental results, the proposed compact disordered structure has a tolerance range for the uncertainty of geometry parameters.

More importantly, due to the universality of the Maxwell's equations in the whole electromagnetic spectrum, we can also design disordered all-dielectric magnetic nanostructures with free space magnetic field enhancement in the visible spectrum. The results are shown in Figure 5(a) and (c), where similar enhancements of magnetic field can be obtained in two plane wave excitation cases. The corresponding normalized distributions of magnetic field $|H_z|$ under the optimized conditions on a plane 10 nm above the structure are shown in Figure 5(b) and (d), where the magnetic field distributions are featured with magnetic hot-spots. It should be pointed out that the optimization of magnetic field enhancement at a targeted frequency could also realized in the procedure of SAA, where the resonant enhancement of the magnetic dipole transition can be anticipated [29]. The above numerical and experimental results validate that the combination of SAA and solutions of Maxwell's equations is capable of

designing disordered nanophotonic structures for enhancing magnetic light-matter interaction. It should be pointed out that we consider the disorder-induced enhancement of magnetic field enhancement in a very compact structure. Ordered structure with sufficient large number of period might outperform the compact disordered one by utilizing the physical concept of quasi-bound state in the continuum.

3 Conclusion

In summary, we propose that compact disordered resonators perturbed from the ordered ones could provide a new degree of freedom for realizing resonant magnetic field enhancement. By combining the SAA with the solution of Maxwell's equations, the automatic design of disordered dielectric magnetic resonators with substantial enhancement of magnetic field in free space is demonstrated. The proposed method is general which is validated by several typical examples in both microwave and optical spectra. The microwave experiment is performed to further strengthen our theoretical proposal. We anticipate our results could shed new light on the ideology of designing all-

dielectric resonant structures for enhancing magnetic light–matter interaction and beyond.

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