Optical Negative Index Metamaterials with Low Losses: Nature-Inspired Methods for Optimal Design

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Abstract: The performance of an optical negative index metamaterial is optimized by simulated annealing, genetic algorithm, and particle swarm optimization methods. While these methods yield very similar designs, the particle swarm optimization shows the best performance.

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1. Introduction

Nano-engineered optical metamaterials (OMMs) have intrigued many researchers due to their novel properties. For example, negative index metamaterials (NIMs) pertinent to perfect imaging [1], do not exist in nature; therefore, they have to be designed and fabricated. Normally, the design of a periodic NIM begins with a 'basis unit cell' providing specific properties to the entire array. A basis 2D NIM unit cell as defined in Ref. [2] and shown in Fig. 1 is used as a starting point, and then adjusted to achieve the best performance. The material properties are limited by the availability of elementary materials; therefore only the dimensions of the basis structure are tuned to find the best performance according to a particular figure of merit. Simulations of different designs are performed using numerical solvers based on periodic finite element-boundary integral method (PFEBI) and spatial harmonic analysis (SHA). Three stochastic optimization algorithms, namely simulated annealing (SA), genetic algorithm (GA) and particle swarm optimization (PSO), then use these solvers to evaluate different design geometries to locate an optimum solution. Because GA is better suited for discrete optimizing parameters it uses the PFEBI solver with uniformly discretized domain for the electromagnetic simulations. SA and PSO utilize continuous parameters and rely on the SHA solver.

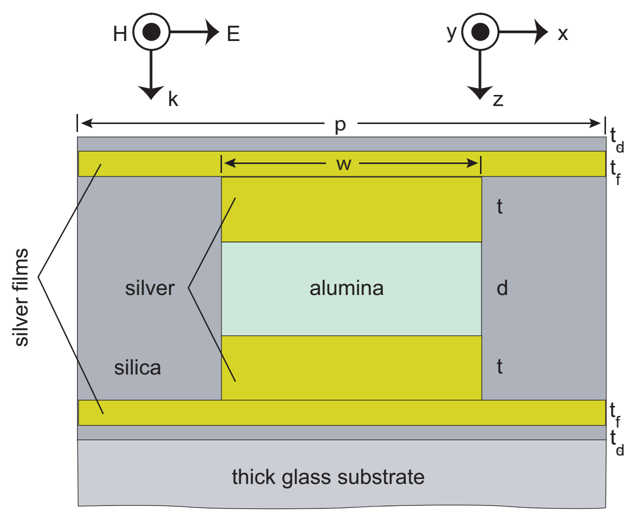

Fig. 1 The unit cell of the NIM geometry

2. Numerical solvers

Periodic Finite Element-Boundary Integral Method (PFEBI)

The PFEBI method is a modified version of the finite element-boundary integral (FEBI) method where periodic boundary conditions have been imposed [3]. In this technique, equations for the unknown electric or magnetic field values inside the computational domain are obtained from the differential form of Maxwell's equations. On the computational boundary, the unknown fields are expanded in terms of known basis functions. The field values from these two computational domains are coupled through integral equations on the boundary.

Spatial Harmonic Analysis (SHA)

SHA is a fast semi-analytic method for simulation of periodic structures [4]. It is based on the expansion of the electromagnetic fields in terms of plane waves as given by Bloch's theorem. The structure to be simulated is divided into layers such that the material properties within a layer are invariant along the direction perpendicular to the layer. The eigenmodes within each layer are expressed as a summation of different plane wave modes as given by Bloch's theorem. The material properties for each layer are expressed as a Fourier series. These substitutions convert the Maxwell's equation into an eigenvalue equation which can be solved to yield the eigenmodes and corresponding eigenvalues for each layer. This is followed by application of boundary conditions at the interfaces between the layers to yield the electromagnetic fields throughout the structure.

3. Optimization algorithms

Simulated Annealing (SA)

SA is formally built upon a physical analogy of cooling crystal structures which spontaneously attempt to arrive at a global minimum [5]. In SA an objective function F is minimized by adjusting a set of parameters. Starting from some point in the parameter space, random move attempts are generated, evaluated, then accepted or rejected according to the change of the objective function F. The acceptance probability is $p = e^{-\Delta F/T}$ for $\Delta F > 0$ and $p = 1$ otherwise. The control variable T ("temperature") is initially set to a high value and then decreased gradually.

Genetic Algorithm (GA)

The GA is based on the principles of natural selection and survival-of-the-fittest in genetic evolution [6]. First, an initial population is formed where each of the 'individuals' corresponds to a specific realization of the design to be optimized in a given parameter space. A cost (to be minimized) or a fitness (to be maximized) is assigned to each individual to quantify its performance. Best-performing individuals in a generation are allowed to 'mate' to produce the next generation of individuals, and a 'mutation' operator is typically introduced to prevent the fitness from converging to local extrema rather than to the global extremum. This process is repeated until convergence is achieved.

Particle Swarm Optimization (PSO)

Swarm intelligence is one of the latest nature-based stochastic optimization techniques, which was recently introduced by Kennedy and Eberhart [7]. Although the driving force behind the GA is competition, the driving force in PSO is cooperation. In a PSO process, particles fly through the multi-dimensional search space with their own position and velocity vectors. A collection or swarm of particles is defined, where each particle is assigned a random position in the parameter space. Based on the fitness (or cost) of the position, each particle moves via a velocity operator until convergence is achieved.

4. Results and Discussions

Four of the geometrical parameters for the NIM are constrained to vary between a minimum and a maximum value (i.e. $50nm \le p \le 500nm$, $20nm \le w \le p$, $20nm \le t \le 60nm$, and $20nm \le d \le 100nm$). The two remaining parameters T_d and T_f are both fixed at 20nm. This choice of T_f is made to guarantee that the silver used in the NIM forms a continuous layer. The figure of merit (FoM) is defined as $FoM = \max_{\lambda}\left(-n'/n''\right)$, where $n = n' + in''$ is the refractive index, and we are interested in the wavelength range $400nm \le \lambda \le 800nm$ with a 10nm interval.

SA: Details and Results

The objective function used in SA is defined as $Obj = 10 - FoM$ since SA requires a positive objective function. Its evaluations were performed by the 2D SHA method. The optimum design obtained by SA is $p = 323.6nm$, $w = 181.6nm$, $t = 40.2nm$, and $d = 80.1nm$ with the effective index $n = -0.83 + i0.22$ at $\lambda = 770nm$, corresponding to a figure of merit 3.79.

GA: Details and Results

The fitness/cost function used in the GA is defined by $fitness = FoM$ and the population size is 6. Fitness evaluations for GA are performed using the PFEBI method. The PFEBI analysis has a basic brick element size of $20nm \times 20nm \times 20nm$, guaranteeing that an element edge would not exceed $\lambda/10$ at any wavelength within the simulation range. The optimum geometrical parameters in this case are found to be $p = 314.3nm$, $w = 176.8nm$, $t = 42.9nm$, and $d = 72.1nm$. The corresponding wavelength is 770nm and the equivalent index of refraction is $n = -0.810 + i0.249$. Convergence to the maximum fitness of 3.25 is achieved at generation 87.

PSO: Details and Results

The cost to be minimized in PSO is $cost = -FoM$. In order to make a fair comparison with the GA, the PSO is started with a swarm of 6 particles and is run for 100 iterations. Fitness evaluations for the PSO are performed by the 2D SHA method. PSO converges to the minimum cost of -3.23 achieved at a wavelength of 780nm with only 35 iterations. The optimized parameters are $p = 328.7nm$, $w = 168.0nm$, $t = 45.8nm$, and $d = 68.0nm$.

The above results show that the optimum designs obtained by the three optimization algorithms are similar, although not exactly the same. Their effective refractive indices (Fig. 2) also confirm this similarity: the three curves almost overlap with each other, featuring a negative index of refraction from 750nm to 810nm.

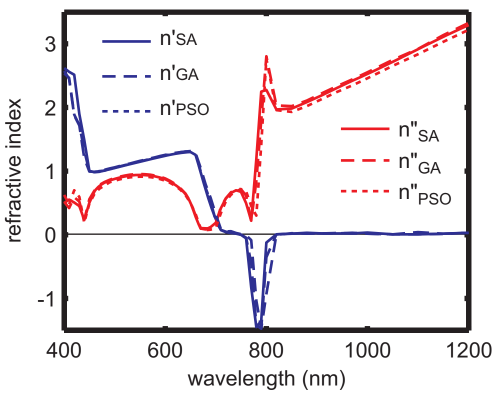

Fig. 2 The effective refractive indices of the optimized designs

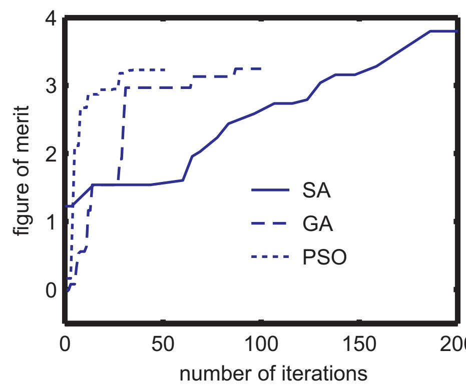

Fig. 3 Comparison of convergence properties of the SA, GA, and PSO optimization methods

Convergence curves for the GA, PSO, and SA methods for this particular optimization problem are compared in Fig. 3. The population size for GA and the number of particles for the PSO are both 6, so each increment in the horizontal axis corresponds to 6 additional evaluations of the fitness function. Because the number of evaluations of the objective function at each temperature for SA is not fixed, we use the total numbers of evaluations of SA divided by 6 as the horizontal axis to make a fair comparison. It is observed that in this particular case the PSO converges much faster than the other two methods.

5. Summary

We have demonstrated the successful optimization of an optical negative index material (NIM) design through three different stochastic optimization tools; genetic algorithms (GA), particle swarm optimization (PSO) and simulated annealing (SA). SA gives a maximum figure of merit 3.79. A maximum fitness (figure of merit) parameter ($-n'/n''$) of 3.25 was obtained through GA after 87 generations, where each generation had 6 individuals. With PSO, a fitness parameter of 3.23 is obtained after only 35 iterations with 6 particles. PSO is found to be the most efficient.

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