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A new optimization algorithm for the design of aperiodic multilayer mirror for 17.1 nm and 30.4 nm

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A new algorithm, Genetic/Tabu hybrid algorithm (GTHA) to optimize the aperiodic multilayer mirrors which combines the advantages of genetic algorithm (GAs) with tabu search (TS) algorithm is proposed in the extreme ultraviolet (EUV) range. Aperiodic multilayers are designed using GTHA for the selection of Fe-IX and He-II emission lines contrasting to the traditional periodic multilayers for a single wavelength. Materials of Mo and Si are selected for their high stability and fairly high reflectivity. High reflectance of 48.62% for the Fe-IX line (λ=17.1nm) and reflectance of 20.57% for the He-II line (λ=30.4nm) are reached by the new algorithm. Comparisons between aperiodic multilayers found by GTHA and the ones optimized using GAs indicate the effectiveness and reliability of the new hybrid algorithm. The aperiodic designs are compared with the periodic ones as well. And the aperiodic multilayers found by GTHA also have the better performance than periodic ones. The practicability of the aperiodic design optimized by GHTA is verified by the sensitivity analyses to thicknesses errors, which indicated it more feasible to fabricate the aperiodic multilayers in practice.

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1. Introduction

Solar images taken simultaneously at different wavelengths in the extreme ultraviolet are widely used [1, 2]. Therefore, dual-function or even multi-function multilayer mirrors with high reflectance are of great interest. For space science in the spectral range of extreme ultraviolet (EUV), a periodic multilayer mirror of Mo/Si is conventionally used for its high stability and fairly high reflectivity [1, 3]. However it can only get a relatively high value of reflectance at a single wavelength. In order to get a dual-function multilayer mirror and fairly high reflectance, new materials, new structure combinations and new design methods such as using aperiodic multilayer mirrors were researched based on the conventional periodic multilayer mirror [4-11].

In this paper, an aperiodic multilayer mirror is considered to select Fe-IX (λ=17.1 nm) and He-II (λ=30.4 nm) radiation. However, the evaluation function of performance of an aperiodic multilayer mirror is a complex function of the index and thickness of each layer with many local minimums. Once the materials are fixed, to find the optimal thickness parameters is the most crucial in designing an aperiodic multilayer mirror.

Here, we proposed a new algorithm, Genetic/Tabu hybrid algorithm (GTHA) to optimize the aperiodic multilayer mirrors. Materials of Mo and Si are chosen and the total number of layers and thickness of each layer are optimized. Genetic/Tabu hybrid algorithm is a combinatorial optimization method to optimize the multilayer structure. It combines advantages of genetic algorithms (GAs) with tabu search (TS) algorithm not only of the ability of global search, but also with fast convergence and local search. Comparison between GTHA and Gas indicate the effectiveness and reliability of the hybrid algorithm. Comparing with the 20-periodic Mo/Si multilayers, a higher reflectance at a single wavelength can achieved with periodic multilayers but at the cost of very low reflectance at the other. And the practicality of aperiodic design is shown by sensitivity analyses to thicknesses errors for the 31-layer aperiodic multilayer mirror optimized using GTHA.

2. Reflectance of a multilayer coating

In designing multilayer, a characteristic matrix method based on the Maxwell equations, has been widely used in combination with a trial-and-error method or an iteration method. And a layer-by-layer design method for soft-X-ray multilayer with the aid of graphic representation of the complex amplitude reflectance in a Gaussian plane has been used widely [7,8].

Assume a multilayer coating consisting of a finite number of homogeneous and isotropic layers. Let the total number of the layers be equal to m. Denote the geometrical thickness of the layers as $d_1, d_2, \cdots, d_m$, and their complex refractive indices as $N_1, N_2, \cdots, N_m$. Let us denote the refractive indices of the substrate and the incident medium as N_0 and N_s respectively.

The characteristic matrix of the multilayer coating can be expressed as:

$$\begin{pmatrix} B \\ C \end{pmatrix} = \prod_{i=1}^{m} \begin{pmatrix} \cos\delta_i & \frac{j}{\eta_i}\sin\delta_i \\ j\eta_i \sin\delta_i & \cos\delta_i \end{pmatrix} \begin{pmatrix} 1 \\ \eta_s \end{pmatrix} \tag{1}$$

The δ_i is known as the optical thickness,

$$\delta_i = \frac{2\pi N_i d_i \cos\theta_i}{\lambda} \quad (i = 1, 2, 3, \cdots, m) \tag{2}$$

Here, θ_i is the wave propagation angle and λ is wavelength of incident wave in the outer space. In the *p*-polarization case $\eta_i = N_i / \cos\theta_i$ while $\eta_i = N_i \cos\theta_i$ for *s*-component of the field.

Then we have the reflectance of the multilayer coating:

$$R = \left(\frac{\eta_0 - C/B}{\eta_0 + C/B}\right)\left(\frac{\eta_0 - C/B}{\eta_0 + C/B}\right)^* \tag{3}$$

Once the thickness d_i and index N_i (i= 1, 2, ⋯, m) is given, the reflectance $R_s(\lambda)$ (Reflectance of *s*-polarized wave) and $R_p(\lambda)$ (Reflectance of p-polarized wave) at wavelength λ is determined. Then we have

$$\bar{R}(\lambda) = (R_s(\lambda) + R_p(\lambda))/2 \tag{4}$$

To evaluate the deviation between the spectral property of the multilayer coating and the expected performance quantitatively, an appropriate evaluation function is required [9]. The optimal parameters of multilayer coating can be obtained by calculating the extreme value of the evaluation function. A function of universal application is used here:

$$F(\boldsymbol{x}) = \sum_{i=1}^{l} \mu_i \left[\bar{R}(\lambda_i, \boldsymbol{x}) - \tilde{R}(\lambda_i)\right]^2 \tag{5}$$

where l is the point number of wavelength to be calculated, $\tilde{R}(\lambda_i)$ is the expected reflectance, μ_i is the weight factor, and $\boldsymbol{x} = [d_1, d_2, \cdots, d_m]$is the thickness parameter of multilayer coating.

3. Material selection and dual-function aperiodic design

For the multilayer mirrors designed in this paper, a material couple of Mo/Si is used for its high time stability under vacuum and atmosphere. And a design with a top layer of silicon is preferable. Because the top layer of silicon will be oxidized when the multilayers exposed to the atmosphere, so it can play a role as a protective capping layer. The optical constants at wavelengths 17.1 nm and 30.4 nm are plotted in Fig. 1 obtained from the Center for X-Ray Optics World Wide Web Server [10].

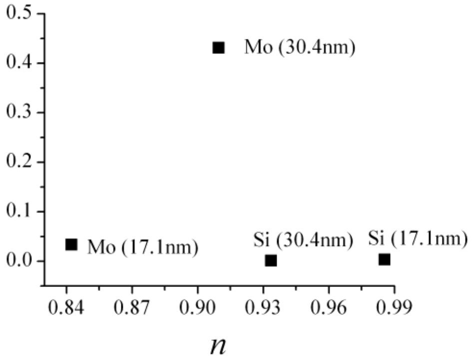


Fig. 1. The complex indices of Mo and Si at the wavelengths of 17.1nm and 30.4nm.

An aperiodic design is adopted in this paper. We attempt to obtain high reflectance at both wavelengths of 17.1 nm and 30.4 nm using thin film interference. And the optical thickness of each layer is used by Genetic/Tabu hybrid optimization algorithm (GTHA) which is described below. The problem to fabricate the aperiodic multilayer mirror is that the aperiodic design may be sensitive to the errors of thickness. In the spectral range of extreme ultraviolet (EUV), the small errors of thicknesses can cause large shift of the spectrum. Fortunately, only two materials of Mo and Si are used in our design，which can effectively reduce the difficulty in fabrication.

Genetic algorithms and Tabu search algorithm are both categorized as heuristic algorithms. Genetic algorithms (GAs) are inspired by the mechanism of evolution and natural genetics. And Tabu search (TS) is a search technique based on the systematic exploration of memory functions. They are generally used because they can easily be engineered to implement any combinatorial optimization problem with good robustness, and all that is required is to have a suitable solution representation, an evaluation function, and a mechanism to traverse the search space. Both the two algorithms are iterative approximation algorithm with a mechanism of randomly search technique, that is to say they do not guarantee finding an optimal solution. Under certain conditions, they asymptotically converge to an optimal solution for their climbing's property. However, each of them has its advantages and disadvantages.

GAs are characterized by a parallel search of the state space as against a point-by-point search by TS as well as the conventional optimization techniques. GAs can solve the combinatorial optimization problem in any high dimensional space, which is independent on the initial solution. Gas have a good global performance for its parallel search. But the problem with genetic algorithms is that they may suffer from premature convergence to a sub-optimal solution. Tabu search enhances the performance of a local search method by using memory structures. It has traditionally been used on combinatorial optimization problems [11,12].

Combining the strengths of the two algorithms, A Genetic/Tabu hybrid optimization algorithm (GTHA) is proposed. A hybrid strategy of genetic algorithms and tabu search has been reported by J. A. Hageman et al. Solutions found by GAs is refined by TS, and a visible transmitting/infrared reflecting filter is given in their design [12]. Here we make GAs as a "main algorithm", and the theory of TS is imported to the reproduction procedure of GAs. The hybrid strategy can described as:

1. The thoughts of "tabu" and "overriding tabu state" are introduced to improve the crossover procedure of GAs. It can not only keep the elite selection structure, but also has the memory structure, which increases genetic diversity and prevents early convergence.

2. Use a Tabu search instead of mutation operation to enhance a local or neighborhood search procedure. Therefore we can get better hill-climbing ability and can avoid premature convergence on poor solutions.

3.1 Initialization

A real-coded schema is adopted in multilayer reflector optimization. A (m+1)-dimensional vector $\boldsymbol{x}$= [m, d_1, d_2, ⋯, d_m] is used to represent the structure parameters of a m-layer coating, with a integer m representing the number of layers in the coatings. The population size NP and the maximum number of generation NG depend on the number of layers, NP=200 and NG=30 for 8-layer coatings for example. The initial population is generated randomly, covering the search space, and then the genes of an individual in the population can be given by:

$$\begin{aligned} &m = m_l + r\cdot(m_u - m_l) \\ &d_i = d_l(i) + r\left[d_u(i) - d_l(i)\right] \\ &i = 1, 2, \cdots, m \end{aligned} \tag{6}$$

Here, r is a random number of [0, 1] (the same later in this paper); m_u, m_l are the maximum and minimum values of number of layers; and $d_u(i)$, $d_l(i)$ are the upper and the lower thickness bounds of i-th layer respectively.

3.2 Selection

The individuals in the population are evaluated by the fitness function that is a measure of how good each individual of current generation is with respect to the desired features. In this problem the fitness function is defined to be:

$$G(\boldsymbol{x}) = 1/F(\boldsymbol{x}) \tag{7}$$

in which F(x) is expressed as formula(5). Use of this fitness function can guarantee that the stronger individuals of current generation have higher fitness values.

3.3 Reproduction

This step is to generate a new generation population from those selected individuals through genetic operators: crossover and mutation.

Crossover: For each pair of "parent" solutions, if $r \le P_c$ (P_c is the probability), the crossover operator is carried out. Two new solutions are created which typically share many of the characteristics of their "parents". The single-crossover is used in this process shown in Fig. 2. The crossover point is produced randomly.

Importing the theory of tabu search, the aspiration criteria equals to the average fitness value of "parent generation", and the tabu target is set to be the individual fitness value. If the new solution is not in the tabu list, it can enter to the next generation. Or else evaluate its fitness, those better than aspiration criteria can override the tabu state and be maintained.

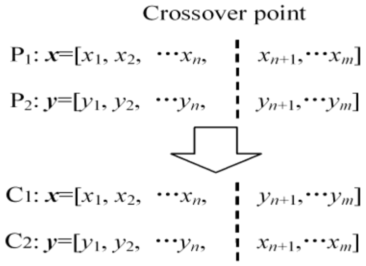


Fig. 2 Schematic diagram of single-point crossover operator in real-coded.

Mutation: In this process a Tabu search in miniature is used. Firstly initialize the parameters of tabu search just as Tabu length, aspiration criteria, and maximum number of iteration. Here the Tabu search is an inbuilt algorithm to enhance local search, so large values of tabu length and number of iteration are unfavorable.

For each individual, if $r \leqslant P_m$ (P_m is the mutation probability), the mutation operator is carried out. Else the process continues to the next individual.

Candidates of appropriate size are "seeded" randomly in areas within a radius of s (s is the minimum distance from current solution to the boundary of search space) of the current solution, expressed in mathematical formula as:

$$\begin{aligned} &m^{new} = m^{odd} + (-1)^{b(i)} r s_m \\ &d_i^{new} = d_i^{odd} + (-1)^{b(i)} r s_i \\ &i = 1, 2, \cdots, m \end{aligned} \tag{8}$$

where $b(i)$ represents the i-th element of the byte that represents the changing direction of genes. For the m-layer coating, there are 2^{m+1} changing directions at most.

Choose the best solution in those candidates according to the aspiration criteria and tabu table, then update tabu table.

If the termination condition of Tabu search is reached, jump out from this loop. Else continue the iterations.

Hereto, a new generation population different from the last one is produced. Generally the average fitness will have increased by this procedure, since only the best organisms from the first generation are selected for breeding, along with a small proportion of less fit solutions, for reasons already mentioned above.

3.4 Termination

The algorithm terminates when a maximum number of generations has been produced, and an optimal solution is to be exported. Or else return to step 3.2 to start a new iteration of propagation with the new generation population.

4. Results and discussion

The briefly described GTHA in Sec.3 is applied to the design of aperiodic multilayer mirrors of for Mo/Si for Fe-IX (λ=17.1nm) and He-II (λ=30.4 nm) radiation operating at normal incidence. Two cases of design problems are discussed: a multilayer mirror with the number of layers between 30~80 and a multilayer mirror with the number of layers is specified to be 40 comparing with a traditional 20-periodic multilayer mirror.

In the first case, the population size *NP* is set to be 1000, the maximum generation number *NG* is 300, the crossover probability P_c equals 0.9 and the mutation probability P_m is 0.2. Additionally, in the mutation process, the tabu length is 20, and the maximum iterative number is 10, for the reasons mentioned in Sec. 3.3. The expectation level is the average fitness value of "parent population".

The multilayer mirror consists of two materials: Mo and Si with a substrate of silicon wafer. We optimized the total layer number and the physical thickness of each layer. Thickness of each layer is limited in 2 ~ 50 nm and the number of layers is optimized in the range of 30~80. The fitness function is set as Eq. (7) where weight factor μ=1. The expected reflectance is $\tilde{R}(17.1nm) = 60\%$ and $\tilde{R}(30.4nm) = 35\%$.

Fig. 3 shows the reflectance spectrum of the aperiodic mirror optimized using Genetic/Tabu hybrid algorithm. A multilayer mirror of 31 layers is obtained by the optimization procedures, and the thickness profile of this multilayer mirror is presented in Fig. 4(a). High reflectance of 42.65% for the Fe-IX line (λ=17.1nm) and reflectance of 27.22% for the He-II line (λ=30.4nm) are reached, which is better than that of the design reported by Gautier et al [13]. The thinnest layer in the multilayer mirror is the 10-th layer: a 2.22 nm-Mo layer. The reflectance of an aperiodic multilayer mirror optimized using traditional GAs is presented for comparison (Fig. 3 dashed line) and the thickness of each layer is showed in Fig. 4(b). The mirror found by GAs consists of 51 layers. It apparently shows that GTHA returns a solution with better spectrum quality and the solution found by GTHA consists of less layers and has a smaller total thickness of 236.92 nm. A simpler structure can greatly decrease the difficulty in fabricating. So we can come to the conclusion that GTHA returns a solution much better than the one found by traditional GAs.

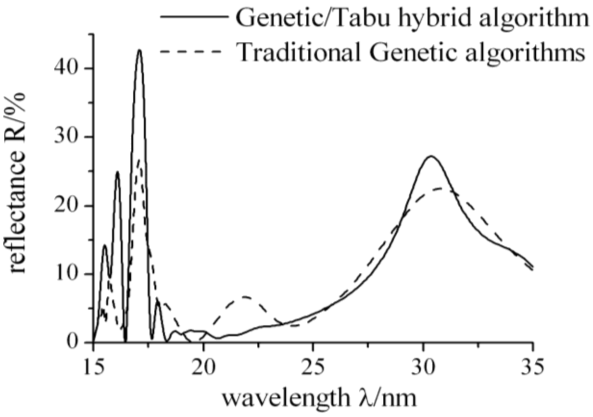
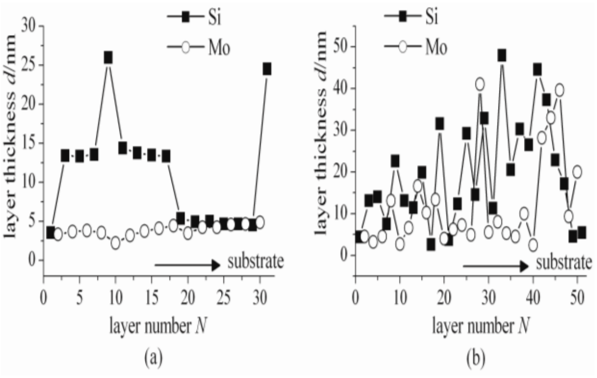


Fig. 3. Reflectance of aperiodic mirror optimized using GTHA and traditional Gas.



(a) (b)

Fig. 4. Thickness profiles of the aperiodic multilayer mirrors optimized using GTHA (a) and GAs (b) with the total number of layers limited in the range of 30~80.

In the second case, the number of layers is fixed to be 40 in order to compare with a traditional 20-periodic multilayer mirror. The population size *NP* is set to be 800, and the maximum generation number *NG* is 200 for the smaller searching space in this case. Other parameters keep the same.

The comparison of the 40-layer aperiodic multilayer optimized by GTHA and the one optimized by traditional GAs is presented in Fig. 5. All the parameters initialized the same. The thickness profiles of the aperiodic multilayer mirrors are shown in Fig. 6. High reflectance of 48.62% for the Fe-IX line (λ=17.1nm) and reflectance of 20.57% for the He-II line (λ=30.4nm) are reached. An obvious improvement is obtained using GTHA.

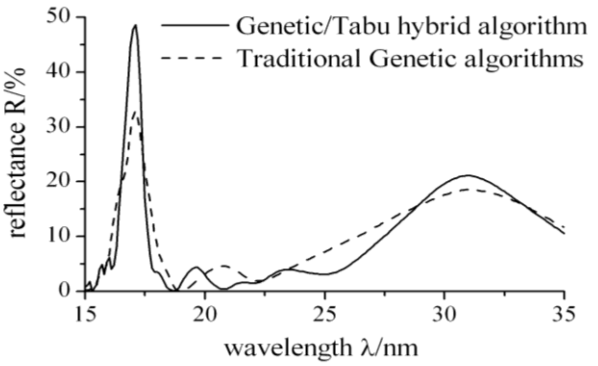


Fig. 5. Comparison of optimized using GTHA and the traditional genetic algorithms.

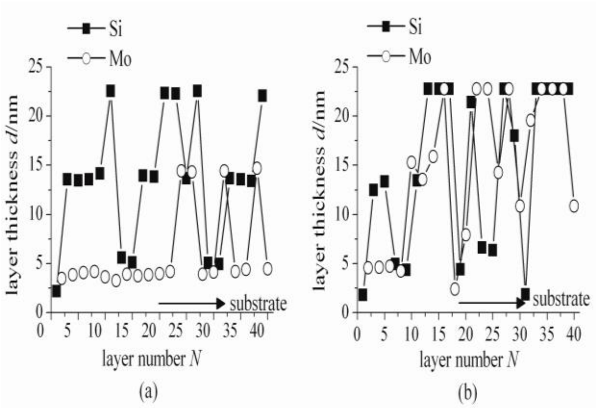


Fig. 6. Thickness profiles of the aperiodic mirror optimized using Genetic/Tabu hybrid algorithm (a) and traditional genetic algorithms (b).

Fig. 7 is the comparison of an aperiodic 40-layer mirror optimized using Genetic/Tabu hybrid algorithm (solid line) with the traditional periodic multilayers (dashed line). The Si/Mo-period of the traditional periodic reflector is 13.39 nm/4.35 nm. It can be clearly seen that the aperiodic multilayer mirror has a better spectrum quality especially at wavelength of 30.4 nm.

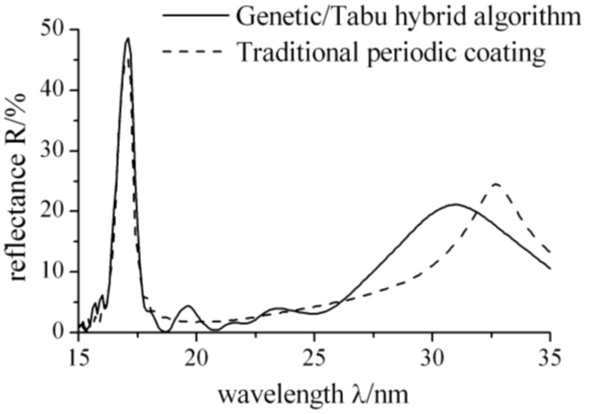


Fig. 7. Reflectance of aperiodic mirror optimized using GTHA with the number of layers fixed to be 40.

Following the design of Gautier et al [13], an analogous structure of dual-periodic design with two but not three material is optimized using simplex optimization method. This dual-periodic design consists of two 10-period multilayers whose thicknesses of Mo/Si pair are 3.84/13.6 nm and 3.61/5.40 nm respectively. It has an analogous spectrum curve (shown in Fig. 8 in dashed line) with that of one periodic design. Better performance of the aperiodic multilayer mirror optimized using GTHA can be seen especially at wavelength of 30.4 nm.

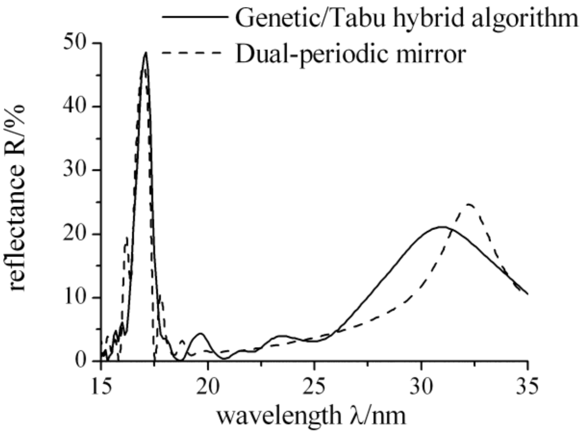


Fig. 8. Comparison of the aperiodic multilayer mirror optimized using GTHA and an optimal dual- periodic multilayer mirror.

Obviously, the Genetic/Tabu hybrid algorithm can get a better result with the same parameters. The periodic designs can easily get a relatively higher reflectance at 17.1 nm but a low reflectance at 30.4nm. A high reflectance at 30.4 nm is obtained at the expenses of a very low reflectance at 17.1 nm. The designs optimized using GTHA perform better than that developed by Julien Gautier et al because we use only two materials Mo/Si instead of B_4C/Mo/Si.

It is interesting to be seen in Fig. 4 and Fig. 6 that the GTHA method resulted in essentially several unique thicknesses for layers (near 4nm, 14 nm and 24nm but not the upper and lower bounds we set) while the traditional GAs has a wider spread in thicknesses. Comparing these designs presented above it may just indicate that for the expected spectrum characteristic in this paper, the solutions with several special thickness values are preferable. And it also illustrates that the GTHA method returns a relatively better solution than GAs. The reliability of the hybrid algorithm can be seen.

Actually, different designs will be returned every time we run the optimization because of the randomly search of the algorithm. If the *NP* and *NG* are big enough, the algorithm will converge on the global optimum solution. However we will come to the same conclusion with the parameters of limited values.

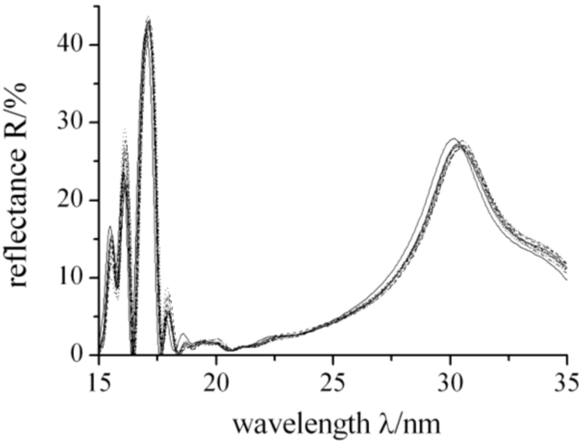


Fig. 9. Sensitivity analyses to thicknesses errors for the 31-layer aperiodic multilayer mirror optimized using GTHA.

At last, sensitivity analyses are conducted to thicknesses errors for the 31-layer aperiodic multilayer mirror optimized using GTHA. Normally distributed errors are introduced into the thicknesses of layers. The mean error is 0 and the standard deviation is 0.1nm that most of coating machines can achieve this accuracy. Ten curves of reflectance are calculated and plotted in Fig. 9 The reflectance for the Fe-IX line (λ=17.1nm) is ranged in 40.21%~43.69 and for the He-II line (λ=30.4nm) the reflectance is ranged from 26.56% to 27.59%. It indicates that the multilayer mirror is robust to the errors of thicknesses of layers, and it will be not too difficult to be fabricated practically.

5. Conclusion

For extreme ultraviolet imaging of the solar corona by reflecting the Fe-IX (λ=17.1nm) emission line and He-II (λ=30.4nm) emission line, we designed the aperiodic multilayer mirrors of Mo/Si using Genetic/Tabu hybrid optimization algorithm which proposed in this paper. Number of layers and thicknesses of each layer are optimized using GTHA and GAs. A 31-layer aperiodic multilayer mirror of Mo/Si is found by GTHA method. High reflectance of 42.65% for the Fe-IX line and reflectance of 27.22% for the He-II line are reached. 40-layer aperiodic multilayer mirrors are optimized using GTHA and GAs to compare with the 20-periodic Mo/Si multilayers. Comparison between GTHA and GAs indicate the effectiveness and reliability of the hybrid algorithm. Comparing with periodic multilayers, an improvement of 3.57% reflectance for the Fe-IX line and 8.18% reflectance for the He-II line is obtained. A higher reflectance at a single wavelength can achieved with periodic multilayers but at the cost of very low reflectance at the other. And the practicality of aperiodic design is shown by sensitivity analyses to thicknesses errors for the 31-layer aperiodic multilayer mirror optimized using GTHA.

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