Application of Luus-Jaakola optimization method to the design of optical coatings

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Abstract: Designing multilayer optical coatings is a difficult optimization problem because of the huge size of the search space. In the present paper, the Luus-Jaakola (LJ) optimization procedure, a new optimization algorithm, is employed to model multilayer optical coatings in the X-ray domain. With this algorithm it is not necessary to specify initially the number of layers present in a design. Only an upper limit needs to be defined. The algorithm has been used to maximize the reflectivity over a range of incident angles at a fixed wavelength, and over a wavelength range at a fixed incident angle. We have also optimized multilayer mirrors of platinum-carbon layer pairs for the hard X-ray region at different grazing angles. The results show that the LJ algorithm can be effectively applied to the design of multilayer optical coatings resulting in fewer layers than obtained using alternative optimization methods.

Key–Words: Luus-Jaakola optimization, Multilayer mirrors, Reflectivity, Hard X-ray optics

1 Introduction

The Luus-Jaakola (LJ) optimization procedure [1] has enabled several difficult optimization problems to be solved, including the solution of a wide variety of problems in optimal control, such as singular time optimal control [2]. This optimization procedure has been used effectively for the optimization of complex systems such as heat exchanger networks [3], and it has successfully been employed for the minimization of the Gibbs free energy for single phase situations [4]. The LJ method and Genetic algorithm have been compared [5]. It was found that the LJ method is faster and is more reliable in achieving the global optimum.

Luus [6] suggested using a multipass procedure in order to improve the convergence rate. If, in a given iteration, the range is smaller than some tolerance ϵ, then the region size would be set equal to that tolerance. The goal of this paper is to test the reliability of the LJ optimization procedure by optimizing the reflectivity profile of multilayer coatings both over a range of wavelengths at a fixed incident angle, and over a range of incident angles at a fixed wavelength. The LJ method also has the advantage of allowing the number of layers in the mirror to be one of the variables that can be optimized.

2 Multilayer Reflectivity Calculation

A basic understanding of multilayer structures for X-ray and extreme-ultraviolet (EUV) optics has grown significantly in the last decade. Multilayer structures based on X-ray and EUV optical systems are in an advanced stage of development in many laboratories. In most of these systems the basic requirements are the highest possible reflection efficiency, moderate energy resolution and high-imaging characteristics. Therefore, to increase the reflection efficiency, periodic multilayers are prepared as artificial structures, where not a single surface, but many interfaces reflect the incoming beam. At an appropriate angle of incidence, the beams reflected from individual interfaces combine together in phase to produce an intense reflected beam.

A multilayer coating for X-ray mirrors consists of a stack of alternating layers of two materials: an absorber and a spacer. The reflectivity of the multilayer coating depends on several parameters: the pair of materials used, the d-spacing, the thickness ratio, the number of bilayers, and the root-mean-square interface roughness.

If the multilayer optics coatings can be considered as a stratified continuous medium, we may use the optical method to calculate its reflectivity. In this approach, a complex refractive index $n = 1-\delta-i\beta$ is at-

tributed to each layer, where δ and β are, as usual, the refractive decrement and the absorption coefficients respectively. We calculate δ and β from the atomic scattering factors f_1 and f_2 using well known relationships, $\delta = Kf_1$ and $\beta = Kf_2$, with

$$K = \frac{r_0 \lambda^2 N_A}{2\pi A}\rho \tag{1}$$

Here r_0 is the classical electron radius, N_A is Avogadro's number,λ is the photon wavelength, A is the atomic weight and ρ is the mass density. The optical constants for the materials are entered from external files which can be loaded from a database [7].

The reflectance of a multilayer system, consisting of N layers can be calculated using a recursive formalism given by Parratt [8]. For s-polarized radiation, where the electrical field vector is perpendicular to the plane of incidence, the Fresnel coefficient for reflection from the interface between the j and $j+1$ layers is given by

$$F_j = \frac{k_j - k_{j+1}}{k_j + k_{j+1}} \tag{2}$$

and for p-polarized radiation, where the electrical field vector is parallel to the plane of incidence it is

$$F_j = \frac{k_j n_j^{-2} - k_{j+1} n_{j+1}^{-2}}{k_j n_j^{-2} + k_{j+1} n_{j+1}^{-2}} \tag{3}$$

with $k_j = \frac{2\pi}{\lambda}\sqrt{n_j^2 - \cos^2\theta_0}$. Here θ_0 and λ are the incident angle and its wavelength respectively. The recursion relation for reflection is given by:

$$R_j = e^{-2ik_j d_j}\frac{R_{j+1} + F_j}{1 + R_{j+1}F_j} \tag{4}$$

where d_j is the thickness of j^{th} layer. The calculation takes into account the decrease of the specular reflectivity due to the interfacial roughness by the modification of the Fresnel coefficients according to

$$F_j = F_0 e^{2k_j k_{j+1}\sigma_j} \tag{5}$$

where F_0 is the reflection coefficient from an ideal interface for either s or p polarization and σ is the root mean square deviation of the interface atoms with respect to a smooth interface. Thus, the procedure to compute the net reflection R_0 coefficients for the multilayer stack is to apply equation 4 recursively, starting at the bottom layer with the assumption that $R_N = 0$, since there is no reflection from an infinitely thick substrate. The final reflectivity from the multilayer system can by obtained from $|R_0|$. For unpolarized radiation the reflectivity is given by the average value of the two polarizations. Finally, the desired spectral reflectance profiles are fitted by minimizing a suitable merit function that is composed of an appropriate function of R defined within the wavelength range or incident angle range. For that we can define the typical figure of merit (FOM):

$$FOM = \sqrt{[\frac{1}{N}\sum_{i=1}^{N}(R(\lambda_i) - R_{des}(\lambda))^2]} \tag{6}$$

3 The LUUS-JAAKOLA (LJ) Algorithm

Let us now consider an optimization procedure that does not require any auxiliary variables to be introduced in order to solve the above parameter estimation problem. The set of variables in the optimization process are described by a vector x consisting of a set of real numbers. The idea of the optimization is then very simple, so the standard LJ algorithm may be summarized most conveniently in the following [5]:

1. Choose some reasonable initial point x^*; a reasonable initial region size r; and choose the number R of random points to be used at each iteration; and the number of iterations M to be used in a pass.

2. Choose R test points through the equation $x = x^* + Dr$ where D is a diagonal matrix of randomly chosen points from the interval [-0.5, 0.5], and r is the region size vector.

3. Check each of the R test points with respect to feasibility from the domain of variables.

4. For each feasible point evaluate the FOM as given by eq.(6)

5. Replace x^* by the test point that gives the smallest value for the FOM.

6. Repeat steps 2-5 for M iterations.

7. Reduce the region size vector r by γ through $r^{j+1} = \gamma r^j$ where γ is a region contraction factor such as 0.95, and j is the iteration index.

8. Go to step 2 and continue for M iterations to finish a pass and examine the results.

The modification of the LJ optimization procedure for multilayer optics coatings may be given by the followings steps:

1. Choose a reasonable initial number of layers ι^*,for example $\iota^* = 0.5(l_{max} + l_{min})$, where l_{max} is the maximum number of layers and l_{min} is the minimum number of layers allowed.

2. Choose a reasonable initial region size for the number of layers r_{layer}, for example $r_{layer} = 10(l_{max} - l_{min})$.

3. Choose some reasonable initial thickness d^*, for example $d^* = 0.5(d_{min} + d_{max})$, where d_{min} is the minimum thickness and d_{max} is the maximum thickness.

4. Choose a reasonable initial region size r, for example $r = 4(d_{max} - dmin)$.

5. Choose the number R of random points to be used at each iteration; the number of iterations M to be used in a pass; and the number of passes Q.

6. Choose a test point R through the equation $\iota = \iota^* + Dr_{layer}$ where D is a diagonal matrix with randomly chosen elements from the interval [-0.5, 0.5].

7. Check each of the R test points with respect to feasibility with the domain of layers.

8. For every R points, choose the thickness point through the equation $d = d^* + Dr$.

9. Check each of the R test points with respect to feasibility for the domain of thicknesses.

10. For each feasible point evaluate the FOM as given by eq.(6)

11. Replace ι^* by the test point that gives the smallest value for the FOM.

12. Replace d^* by the test point that gives the smallest value for the FOM.

13. Repeat steps 2-12 for M iterations

14. Reduce the region size vector r by γ through $r^{j+1} = \gamma r^j$ where γ is a region contraction factor of thicknesses such as 0.95, and j is the iteration index; reduce the region size for the number of layers by $r_{layer}^{j+1} = \alpha r_{layer}^j$, where α is a region contraction factor for layers, such as 0.96.

15. Go to step 6 and continue for M iterations to finish a pass.

16. At the end of the pass determine the region size to be used at the beginning of the next pass from the size of the variation of each variable as suggested by Luus [5], i.e., choose

$$r_i^{k+1} = |d_i^*(k) - d_i^*(k-1)|, i = 1, 2, ..., N \quad (7)$$

where $d_i^*(k)$ is the best value of d_i after k passes and $d_i^*(k-1)$ is the best value of d_i after $k-1$ passes and N is the number of layers. If the region size as calculated from equation (7) is less than the region collapse parameter ε, set the region size at the beginning of the pass for that variable equal to ε .

17. If r_{layer} is less than some parameter η put the region size for the next pass equal to some integer value, for example 10.

18. Continue the procedure for Q passes.

19. Run the algorithms many times and examine the results.

4 Examples and Numerical Results

Initially the algorithm was used to design multilayer stack structures for high reflectivity in the wavelength range 16-19 nm at normal incidence. Note that for X-ray mirrors this is a sufficiently wide range of wavelengths. On the one hand it is required that the mean reflectance in the target wavelength range is a high value, wherever possible. On the other hand it is also desirable to have the smallest possible number of layers. It is also required that variations of the reflectance from the mean value in the target wavelength be small enough.

Along with the above target demands there are a number of additional feasibility demands. The thicknesses of each layer should be in the range from 0.8nm to 12nm. Also the roughness was taken to be $\sigma = 0.3nm$.

The layer materials were chosen to be Mo and Si, which are known to be suitable materials for the construction of high reflectivity mirrors in this region of the soft x-ray spectrum. For the absorber we have selected Mo and the spacer is Si. The multilayers consist of alternating absorber and spacer layers. The target reflectances for the wavelength region from 16-19 nm were chosen to be 0.2, 0.25 and 0.3. The optimization process adjusts the thickness of each layer, as well as the total number of layers in the stack, in order to achieve the best value for the FOM.

The results are shown in Figure1. The design values for the reflectivity R_0 are 0.2, 0.25 and 0.3, respectively. The reflectance shown in Fig.1 for

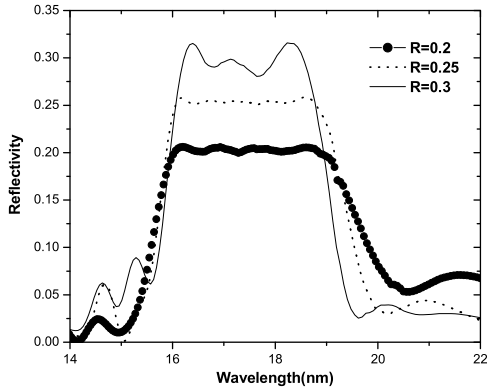

Figure 1: Optimized reflectivity of broadband multilayer mirror Mo/Si in the wavelength range from 16 nm to 19 nm for design $R_0 = 0.2$, $R_0 = 0.25$ and $R_0 = 0.3$

$R_0 = 0.20$ was achieved with a stack having 22 layers. Its reflectance features an excellent uniformity (ΔR=0.002). The best results were achieved with a 32-layer stack for $R_0 = 0.25$. The mean reflectance ($\overline{R}$=0.252) in this case is very good, but the reflectance uniformity in the target region is slightly worse than in the previous case (ΔR=0.004). Also, Fig. 1 shows that the response is less uniform when $R_0 = 0.3$ and more layers were required to achieve the desired reflectivity (34 layers).

The effectiveness of the LJ optimization procedure is confirmed by comparing the above results with those of other authors. Table 1 presents the reflectance of Mo/Si mirrors from ref [9] in the same wavelength range. The number of layers, mean reflectance values, and deviations are compared. For the first case (R_0 = 0.2), the mean reflectance is the same as the result from our LJ calculation, however the uniformity in our case is much better than obtained in ref [9]. In the second case (R_0 = 0.25), the LJ method gives an excellent result for both the mean reflectance and the deviation from the mean. The average reflectivity in the R_0 = 0.3 case is much better than in ref [9]. In all three cases the LJ calculations led to better results with far fewer layers. We reduced the number of layers by 64% in the first design, whereas in the second and third designs they were reduced by 50%.

The LJ optimization procedure was also tested by applying it to design multilayer stack structures for high reflectivity in the energy range 20-40 keV over a range

Table 1: Parameters of multilayer mirror Mo/Si for normal incidence with rms roughness 0.3nm

Design	No. of layers		$\overline{R}$		ΔR	
	Ref. 7	LJ	Ref. 7	LJ	Ref. 7	LJ
0.2	60	22	0.20	0.20	0.04	0.002
0.25	60	32	0.225	0.253	0.08	0.004
0.3	60	34	0.23	0.288	0.14	0.027

of incident angles from 0.1 to 0.358 degrees. The calculations were divided into 13 groups according to the grazing angle. For all mirror groups, the interfacial roughness of two materials is estimated to be 0.3 nm.

The layer materials were chosen to be Pt and C, which are known to be suitable materials for the construction of high reflectivity mirrors in this region of the hard x-ray spectrum [10, 11]. Both materials have no absorption edges in the hard x-ray region concerned. Long term chemical stability and its ease of thin film deposition are also preferable characteristics of platinum. For the absorber we have selected Pt while the spacer is C. The optimization process adjusts the thickness of each layer, as well as the total number of layers in the stack, in order to achieve the best value for the FOM.

The optimization results for the Pt/C mirors studied are summarized in Table 2. Figure 2 also shows calculated reflectivities of all groups. From Table 1, the reflectance at incidence angle 0.11^o was achieved with a stack having only 10 layers. Its reflectance demonstrates excellent uniformity (delta R=0.006). At incident angles of 0.123^o and 0.135^o , the average reflectivities are above 80% and the standard deviation is less than 4% while the numbers of layers required are less than 20. At incidence angles between 0.152^o and 0.187^o, the standard deviations are the same (Δ R=0.09) and the average reflectivity is more than 60%. However, the number of layers are increased up to 28 in order to achieve the higher reflectivity. The angles chosen for these calculations are the same as those used by other authors ref[12]. Even though the critical angle for Pt is 0.161^o, the inclusion of absorption and the roughness at the interfaces results in non-perfect reflection at angles below this.

When the gazing angle is more than 0.2^o, the reflectance uniformity in the target region is less than for the smaller angles. The average reflectivity is in the range 30% to 55% , and the number of layers needed is between 40 and 60. For angles larger than 0.3^o, the reflectivity becomes less uniform and more layers are required to achieve a higher reflectivity (more than 68

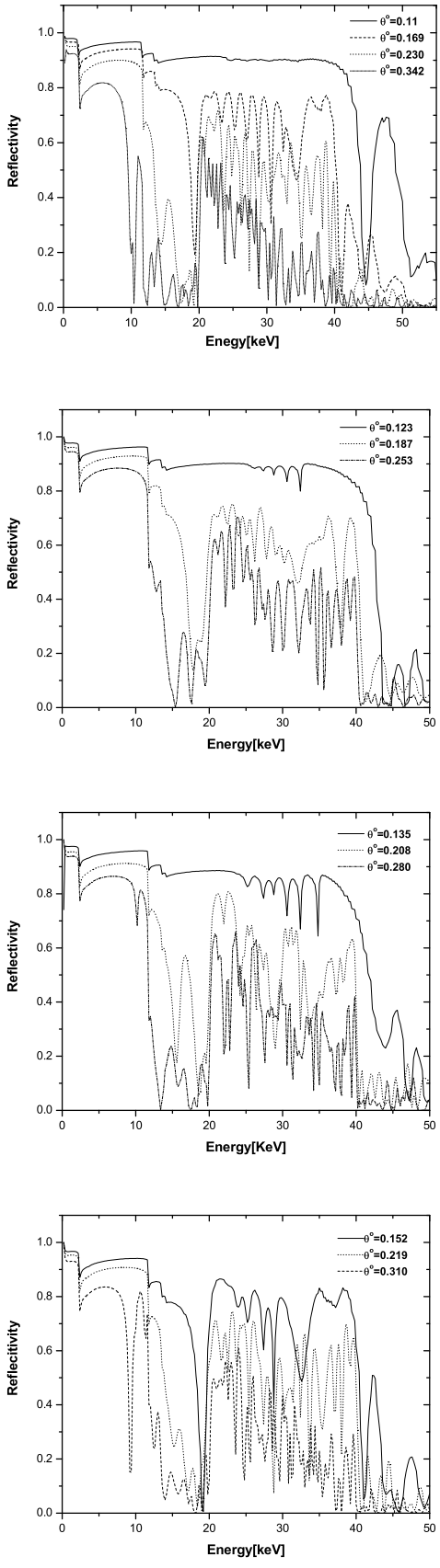

Figure 2: Optimized reflectivity curves of broadband multilayer mirror Pt/C in the energy range from 20 keV to 40 keV at grazing angle from 0.11 to 0.342.

Table 2: Pt/C Mirror design for broad band energy 20-40keV

Group (θ^o)	**Total number of layers**	**total d(nm)**	**Average Reflectivity**	**Standard Deviation**
1	0.11	10	52.1	0.90	0.006
2	0.123	14	87.8	0.88	0.02
3	0.135	18	92.3	0.83	0.04
4	0.152	18	86.2	0.75	0.09
5	0.169	24	108.3	0.69	0.09
6	0.187	28	110.7	0.62	0.09
7	0.208	42	203.9	0.55	0.139
8	0.219	44	176.5	0.532	0.140
9	0.23	46	181.1	0.492	0.133
10	0.253	50	182.4	0.422	0.1355
11	0.28	60	231.5	0.345	0.156
12	0.31	68	241.3	0.28	0.151
13	0.342	76	270.3	0.241	0.156

layers).

The performance parameters of these figures are compared with results from ref[12]. Table 3 presents the reflectance of Pt/C mirrors from ref [12] in the same energy range. The number of layers, mean reflectance values, and total thicknesses of the stack are compared. From grazing angles 0.11^o to 0.187^o , the mean reflectance obtained using the LJ procedure is higher than that found in ref [12] and requires fewer layers. It also results in a reduced total thickness of the stack. For example, at 0.123^o, the LJ method gives a higher reflectivity (by more than 8%)and requires fewer layers (70% less). In addition, the total thickness of the stack is reduced by 40%. However, when the grazing angle is larger than 0.2^o, then the total thickness of the stacks in ref [12] is less than that found using the LJ method. However the LJ result yields a higher average reflectivity and a reduced number of layers. Also, in the LJ method, at 0.28^o, the average reflectivity is increased by 70% over that of ref [12] while the total thickness is also larger by more than 30%.

5 Conclusion

The Luus-Jaakola optimization procedure proves to be a very successful optimization scheme for the design of multi-layer mirrors. Like the Genetic Algorithm (GA), and other stochastic methods, no derivatives of

Table 3: Comparison between LJ method design and ref[12] design of Pt/C mirrors for broad band energy 20-40keV

(θ^o)	Number of layers		Average reflectivity		Total d(nm)	
	LJ	Ref [12]	LJ	Ref [12]	LJ	Ref [12]
0.11	10	50	90%	80%	52.1	152.4
0.123	14	50	88%	80%	87.8	152.4
0.135	18	50	83%	75%	92.3	152.4
0.187	28	82	62%	50%	110.7	190.9
0.208	42	82	55%	40%	203.9	188.5
0.28	60	126	34%	20%	231.5	178.9
0.31	68	126	28%	20%	241.3	178.9
0.342	76	130	24%	20%	270.3	217.8

the figure-of-merit function are required. The prime advantage of the LJ algorithm over the GA is that one can mix integer and real variables in the scheme so that the number of layers can be optimized at the same time as the thicknesses of the layers are being adjusted to achieve an optimum reflectivity. This should prove to be a useful tool for this type of design.

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