

Design of Bifunctional XUV Multilayer Mirrors Using a Genetic Algorithm

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February 24, 2000

Abstract

We designed multilayer mirrors for the IMAGE/Explorer mission that were intended to reflect well at 304 Å and poorly at 584 Å. The best designs utilized the novel materials U and Y₂O₃ with Al or Si as spacer layers. The highest design reflectivities were obtained with aperiodic multilayers, although these were too hard to grow in practice. We found these novel designs using a genetic algorithm calling on a database of 43 promising materials with the freedom of aperiodic multilayer stacks.

1 Introduction

The IMAGE/Explorer Mission scheduled to be launched in February, 2000 includes an XUV telescope designed to provide the first direct images of Earth's magnetosphere[1]. The images result from the fluorescence of He II ions trapped in the magnetic field lines and excited by 304 Å light from the sun. From some viewing angles significant background light is expected from 584 Å light from He I in Earth's ionosphere. Other background radiation is filtered by an oxidized aluminum filter supported on a nickel mesh.

To meet the mission objectives, we wanted to design a mirror with a reflectance greater than 20% at 304 Å and no more than 0.2% at 584 Å. The light will be incident on the mirrors at angles between 11° and 18° relative to the mirror normal. This design is challenging both because of the large range of near-normal incidence angles and the dual (reflective/anti-reflective) function. The design is further complicated by the fact that bulk materials tend to be more reflective at 584 Å than at 304 Å.

We did not want to prejudice our search for an optimal mirror design by preselecting multilayer compositions or thicknesses. This left us with a large parameter space we needed to search that included both discrete and continuous variables. We wanted to constrain mirror parameters to those that were

practical and physically reasonable. We found that an adaptation of the genetic algorithm proved superior to other techniques we considered for this particular application.

Dobrowolski and Kemp[2] provide a good survey of alternative techniques for optical design optimization representative of those we considered trying. None of the techniques they mention could be adapted to efficiently optimize designs that rely on discrete unordered parameters (the choice of materials for each layer).

In the next section, we outline the basics of our genetic algorithm implementation. Further details can be found in references [3] and [4]. Section 3 discusses the optimal designs we found. The performance of the final flight mirrors is discussed in Section 4. In Section 5, we discuss the differences between calculated and measured mirror reflectivities and some lessons we learned from these particular multilayer designs.

2 Genetic Algorithm

In optimizing our mirror design, we wanted the freedom to independently vary the thickness of up to 16 layers of two different materials. We wanted our optimization algorithm to also select the materials out of a list of about 40 for the composition of the alternating layers. The function we were optimizing, which we called our merit function, had many local minima. The layer thicknesses varied continuously within constraints, but the selection of materials was a selection among discrete choices. These characteristics called for an optimization algorithm that was global (or at least approximately so), was efficient in a large parameter space, and could work with discrete and constrained continuous variables. Johnson and Rahmat-Samii's success using the genetic algorithm in optimizing antenna designs[5] encouraged us to adapt it for this problem as well. Simulated annealing, a competitive technique with most of the same advantages (at least in principle) has been used by Boudet et al. for other thin-film optics designs[6].

The genetic algorithm models nature's process for optimization and refinement through DNA-encoded traits, inheritance, mutation, and survival of the fittest. The parameters characterizing each multilayer mirror were encoded in chromosomes as shown in Figure 1. The space for each characteristic encoded

Material 1	Material 2	1 A - Thickness 1	2 A - Thickness 2	1 B - Thickness 3	2 B - Thickness 4
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Figure 1: Composition of chromosomes in the genetic algorithm. 1A is the thickness of material 1 in the first layer-pair, 2A is the thickness of material 2 in the first layer-pair, etc.

in the gene is called an allele. The first two alleles of the chromosomes specify which materials are used in the alternating layers of the mirror. The remaining alleles give the thicknesses of the alternating layers in the mirror.

For each gene, a merit function is calculated, assigning a fitness f to each gene. This is the function the algorithm is designed to maximize. In this problem, subtle differences in the choice of a merit function had a dramatic influence on the final solution. Our first choice for f was

$$f = \left(1 - \frac{0.002}{r_{584}}\right) + \frac{r_{304}}{0.2}, \quad (1)$$

where r_{584} is the reflectance at 584 Å and r_{304} is the reflectance at 304 Å. We abandoned Equation 1 and our second choice,

$$f = \frac{r_{304}}{r_{584}}, \quad (2)$$

because they permitted optimal solutions with extremely low reflectivities at 584 Å and only marginal reflectivities at 304 Å. Our best choice for f was

$$f = \frac{r_{304}}{\max(0.002, r_{584})}. \quad (3)$$

The reflectivities were calculated using the Parratt formula[7] and assuming no roughness or interdiffusion at the multilayer boundaries. Both roughness and interdiffusion could easily be incorporated into the merit function if desired.

The algorithm proceeds by first choosing an initial population with random parameters within the constraints we imposed on the problem space. These constraints were that layer thicknesses be between 20 Å and 275 Å and that the layers be composed of one of 43 materials we had pre-selected as reasonable materials for us to sputter. In each succeeding generation, the least fit half of the population are replaced by children derived from parents of the previous generation.

The material choices were selected based on the $\delta - \beta$ plots by Fennimore[13]. In these plots, Fennimore plotted $\delta = 1 - \Re(n)$ on one axis and $\beta = \Im(n)$ on the other axis. Materials were sought that provided the greatest contrast in $\Re(n)$ with minimum absorption (small values of $\Im(n)$).

The parents for the children are chosen by a process called tournament selection. For each parent, two members of the population are chosen at random and their merit functions compared. The most fit of the two is chosen as a parent. After two parents are selected, two children are created from the parents' genes. Each child starts with genes identical to that of one of the parents. These genes are then subject to crossover and mutation.

Crossover is a process where the genetic sequence of a child taken from one parent is interrupted and replaced by that of the other parent. If the break is in the middle of an allele for a continuous parameter, the new allele is an average of the alleles of the two parents. If the break is in the middle of an allele for a discrete parameter, the new allele is a combination of the binary-encoded

Y ₂ O ₃ thickness, Å	Al thickness, Å
44	134
54	110
64	122
61	111
60	118
60	106
74	99
102	79

Table 1: Composition of optimal Y₂O₃/Al stack. The 44 Å Y₂O₃ was on top of the stack where the light hit. The 79 Å Al layer was in contact with the quartz substrate.

material characteristics of each parent. We found that the algorithm converged most quickly using a random crossover probability of 70%.

Allowing random mutations also improved the convergence of the algorithm. We found that selecting a 5% mutation probability was optimal for this problem. In a mutation, a random bit in the chromosome was switched from a '1' to a '0' value. If this resulted in a non-existent material, the mutation was repeated. Any encoded thickness was valid, so the same check wasn't necessary there.

After crossover or mutation, the gene is checked to make sure the parameter values are still within the constraints. If they are not, the child is replaced with a new one.

The process of generation of children continues until the population is full. Half of each new generation will be the most fit parents of the previous generation. The other half are the children generated by the process described above. The process of refining succeeding generations continues until the algorithm converges to a solution. For our mirrors, a population of 10,000 to 20,000 was adequate. Solutions typically converged in 10–15 generations. Details can be found in [3, 4].

Figure 2 is a flow chart summarizing the above steps in the algorithm. A C++ implementation of the algorithm can be found in Lunt's honors thesis[3].

3. Resulting Designs

The best mirror design found by the genetic algorithm was an aperiodic stack of Y₂O₃ and Al grown on a quartz substrate (the choice of substrate did not significantly affect the reflectance). The layer thicknesses are given in Table 1. For Y₂O₃ we used the optical constants $\delta = 0.376$ and $\beta = 0.248$ at 304 Å and $\delta = -0.042$ and $\beta = 0.543$ at 584 Å[9]. For Al we used the optical constants $\delta = 0.0488$ and $\beta = 0.0056$ at 304 Å[10] and $\delta = 0.2851$ and $\beta = 0.0237$ at 584 Å[9]. Figure 3 is the computed reflectance of this mirror at 304 Å as a function of grazing angle. Figure 4 is the computed reflectance of the same

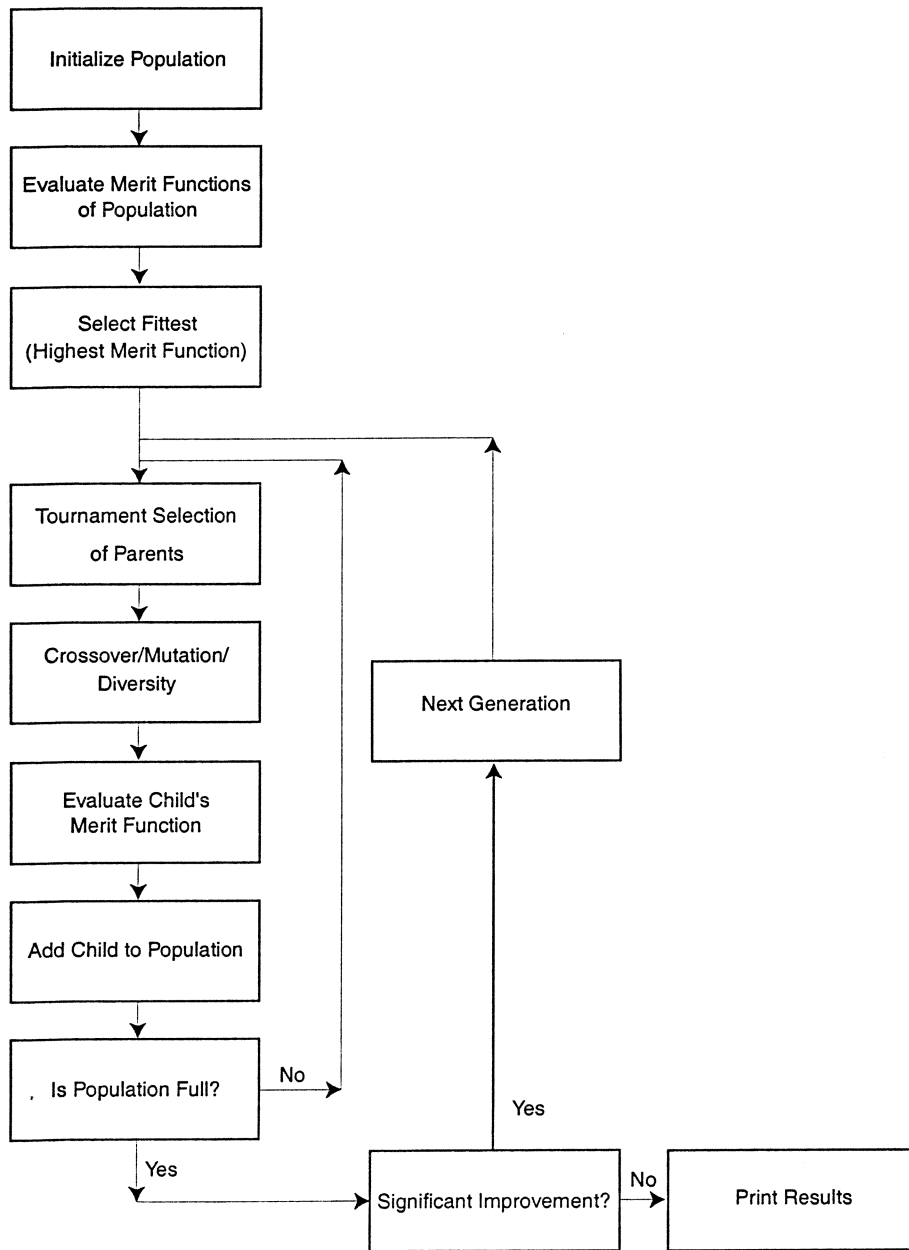


Figure 2: Flow chart of the genetic algorithm

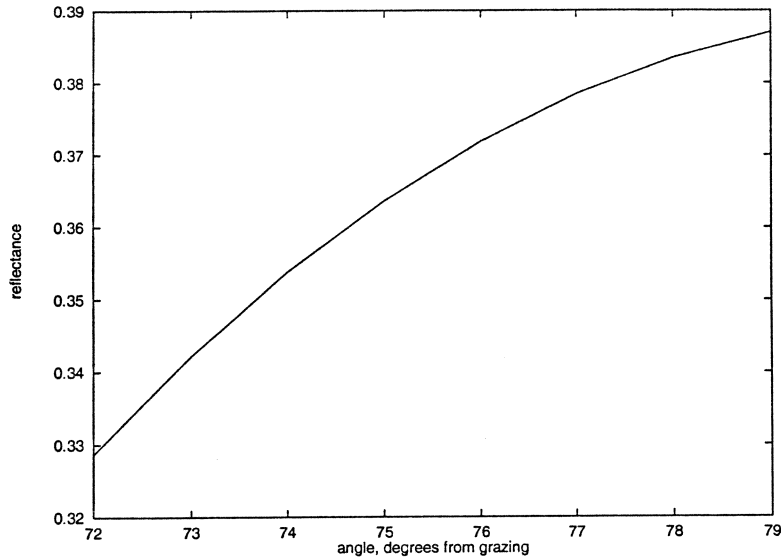


Figure 3: reflectance of the optimum Y_2O_3 mirror at 304 \AA .

mirror at 584 \AA as a function of grazing angle.

There are a couple of uncommon features in this mirror design. The first is that this slightly aperiodic mirror is predicted to have better performance than a strictly periodic one. Secondly, the use of an oxide as the top layer usually greatly reduces the reflectance at 304 \AA , rather than providing relatively high reflectance as seen here. Having yttria as the top layer has the further advantage of serving as a capping layer to prevent the underlying aluminum layer from oxidizing. A layer of Al_2O_3 significantly degrades the performance of the mirror because it is highly absorbing in the extreme ultraviolet.

Because we did not have the facility at the time to produce sputtered Y_2O_3 , we tried eliminating Y_2O_3 from the data base to find the next best choice. The resulting aperiodic uranium/aluminum mirror also had excellent reflectance at 304 \AA but was more reflective at 584 \AA than the Y_2O_3 mirrors. Table 2 gives the layer thicknesses for this design. The optical constants we used for uranium were $\delta = 0.3219$ and $\beta = 0.2798$ at 304 \AA [10] and $\delta = -0.1773$ and $\beta = 0.2947$ at 584 \AA [11]. The predicted reflectivities of this mirror at 304 \AA and 584 \AA are shown in Figures 5 and 6.

This aperiodic design was difficult for us to fabricate because we used near grazing x-ray reflections at the Cu K- α line to measure our layer thicknesses. The irregular patterns produced from aperiodic stacks are much more difficult to interpret than those from periodic designs.

Our best periodic U/Al multilayer design had eight layer pairs of uranium

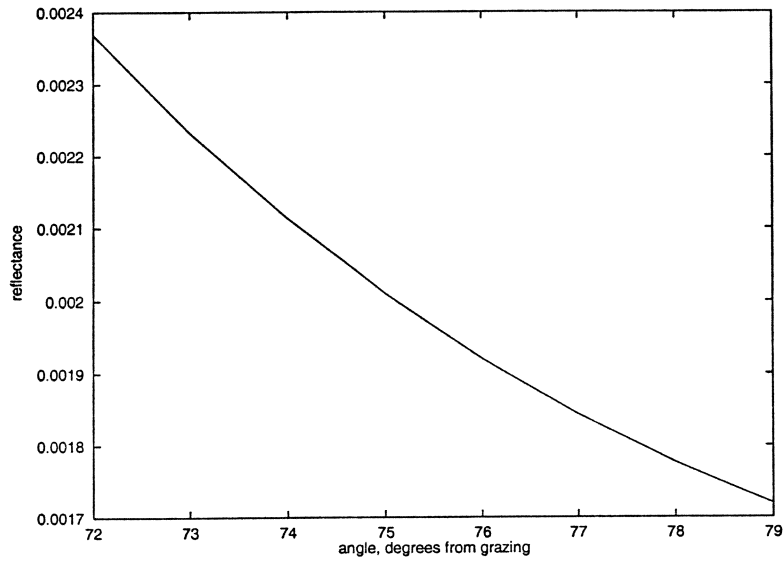


Figure 4: reflectance of the optimum Y_2O_3 mirror at 584 Å.

U thickness, Å	Al thickness, Å
53	129
74	85
124	119
45	81
122	264
218	131
52	219
109	183

Table 2: Composition of aperiodic uranium/aluminum mirror. The 53 Å U layer is the top layer exposed to the light. The 183 Å Al layer is in contact with the quartz substrate.

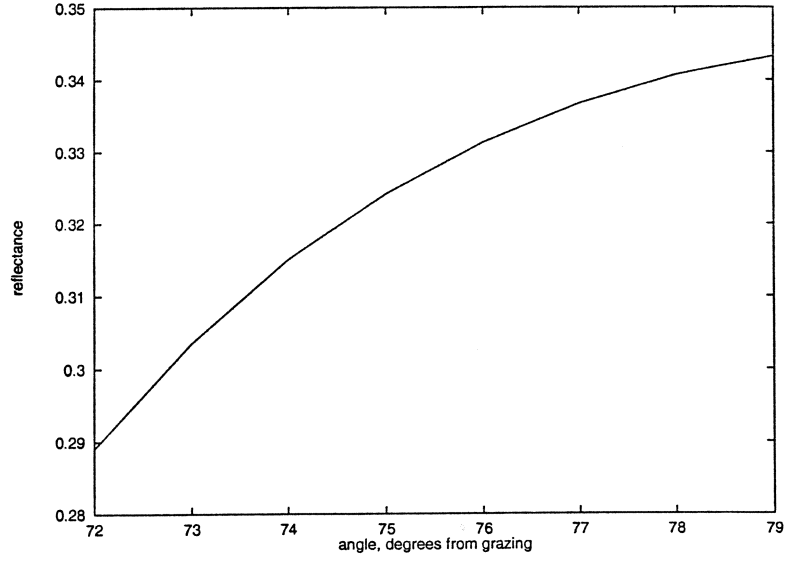


Figure 5: reflectance of best aperiodic U/Al mirror design at 304 Å.

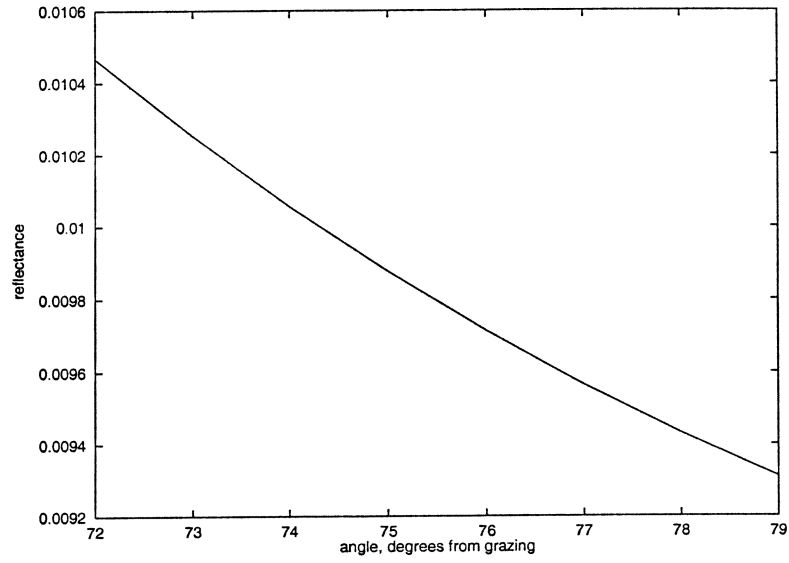


Figure 6: reflectance of best aperiodic U/Al mirror design at 584 Å.

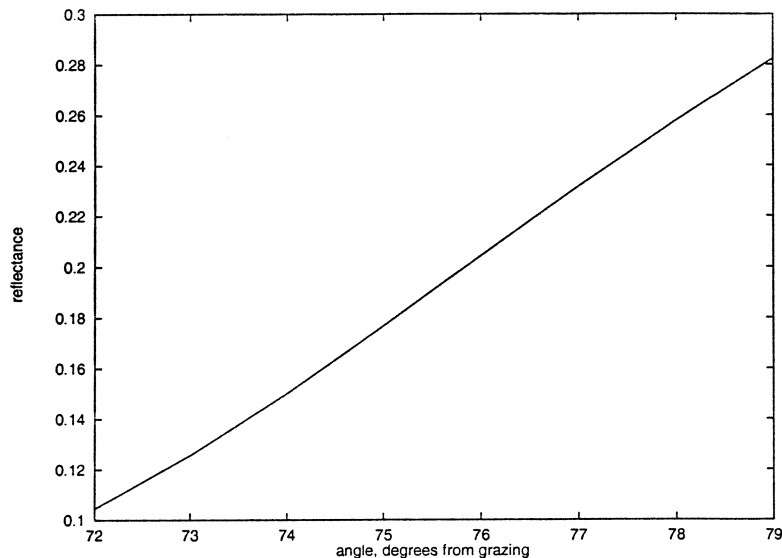


Figure 7: reflectance of best periodic U/Al mirror design at 304 Å.

with thicknesses of 41 Å and aluminum with thicknesses of 129 Å. They were designed using Windt's IMD program[8] and gave the reflectivities shown in Figure 7 and 8. Note the decrease by from about 32% to about 20% in the average reflectance at 304 Å with the periodic design.

The U/Al mirrors had a significant oxidation problem of that led us to abandon this design in favor of U/Si stacks. Our final design was a periodic U/Si stack with seven pairs of 53.6 Å thick uranium and 128.5 Å thick silicon layers. Though the aperiodic designs had higher theoretical reflectance, they proved too difficult to grow. We have not yet developed a reliable technique to measure (and hence control) layer thicknesses in an aperiodic multilayer stack.

The final design was based on the silicon optical constants $\delta = 0.0708$ and $\beta = 0.00907$ at 304 Å[10] and $\delta = 0.20953$ and $\beta = 0.1117$ at 584 Å[9]. These designs had the computed reflectivities shown in Figures 9 and 10. In the next section we will discuss our final fabricated mirrors that are based on this design.

4 Measured Reflectivities

Allred et al. have fabricated mirrors[12] based on the periodic and aperiodic the U/Al designs and the periodic U/Si design. The measured reflectivities of the U/Al designs were much poorer than predicted by theory. Fennimore's analysis indicated that oxidation of the top uranium and aluminum layers was probably

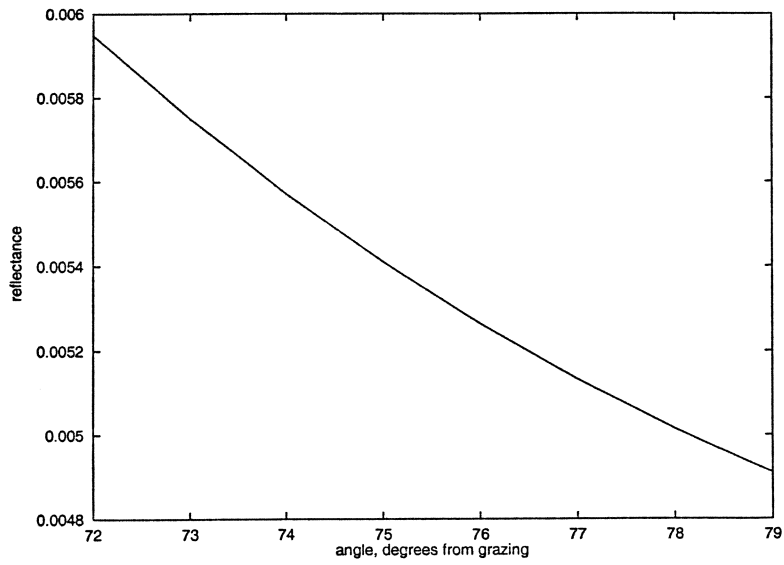


Figure 8: reflectance of best periodic U/Al mirror design at 584 Å.

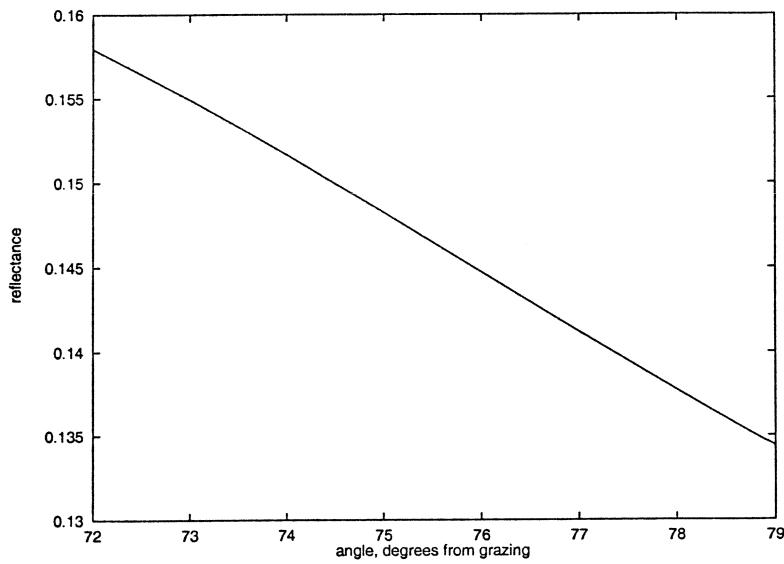


Figure 9: Computed reflectance of optimal periodic U/Si mirrors at 304 Å.

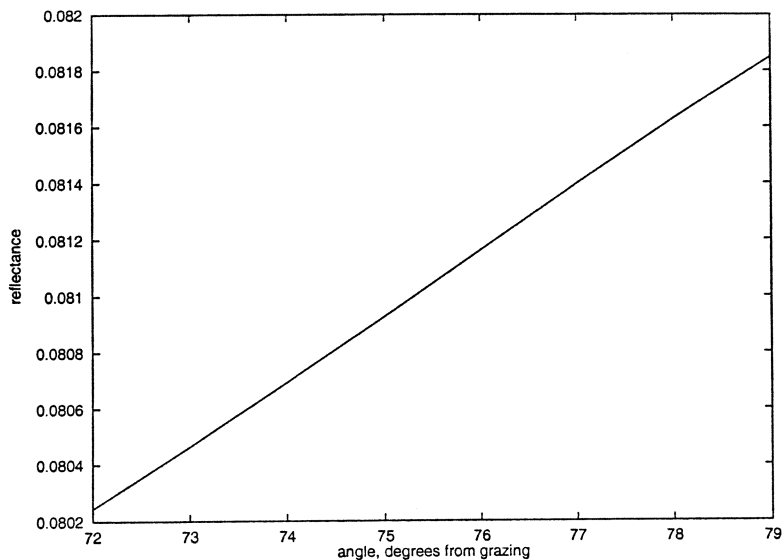


Figure 10: Computed reflectance of optimal periodic U/Si mirrors at 584 Å.

the reason for this degradation[13].

We instead resorted to the U/Si design with a UO_3 cap intended to stop the oxidation of lower layers. The UO_3 layer was produced by sputtering a U layer and letting it oxidize. To our surprise, the cap also dramatically improved the performance of the mirrors, both at 584 Å and 304 Å[12]. The reflectance at 584 Å was reduced from a predicted 8% to a measured 0.84%. The reflectance at 304 Å was raised from a predicted 15% to a measured 17%. We have so far been unable to account for these reflectivities using any reasonable combinations of expected oxide thickness and optical constants. Rowland has made some preliminary new measurements of the index of refraction of oxidized sputtered uranium that indicate it may have an anomalously high real part of the index of refraction[14].

We also tried using a SiO_2 cap produced by sputtering a top layer of Si and letting it oxidize. All of the mirrors we produced with SiO_2 caps had significantly degraded optical performance.

5 Conclusions

An adaptation of the genetic algorithm has proved to be a robust technique for designing aperiodic bifunctional multilayer mirrors in the soft x-ray and extreme ultraviolet wavelengths. The algorithm successfully finds optimal designs with

the freedom to select both multilayer materials and layer thicknesses. Using this algorithm, we discovered several designs using two materials that have not frequently been used as optical materials at these wavelengths in the past, Y_2O_3 and U.

The most promising materials for growing multilayer mirrors with near-normal high reflectance at the He II line at 304 Å and low reflectance at the He I line at 584 Å are Y_2O_3 with an Al spacer layer. The aperiodic mirrors we designed had a reflectance greater than 30% at 304 Å and about 0.2% at 584 Å. We were unable to fabricate these mirrors using DC magnetron sputtering because Y_2O_3 is a ceramic insulator. With the installation of an RF sputtering system, we hope to be able to fabricate one in the near future.

Uranium/aluminum mirrors also promise high reflectance at 304 Å, though they are not as good at rejecting light at 584 Å. Their performance degrades rapidly with oxidation of the top U and Al layers.

Uranium/silicon mirrors were adequate and the most practical ones for our application in the IMAGE/Explorer mission. For reasons we do not yet understand completely, capping these mirrors with a UO_3 layer significantly improved their lifetime and performance.

Aperiodic designs can significantly improve the performance of the types of bifunctional mirrors we needed for our application. Experimental techniques to monitor sputtered layer thicknesses need to be developed before they can be practical however.

6 Acknowledgements

We wish to thank Adam Fennimore, Matt Squires, David Balogh, Spencer Olson, Jim Thorne, Greg Harris, Ross Robinson, and Charles Curtis for their assistance in growth, design, and characterization of our mirrors.

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