

# Study of Potential Quantization Effects in Designs for 12.4 nm Mirrors

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## ABSTRACT

Mirrors at normal incidence have been successfully made for the 12.4 nm spectral region using molybdenum (Mo), silicon (Si), and other materials. At these wavelengths, a typical layer is of the order of 3 nm in physical thickness, and the atomic diameters of the materials are of the order of 0.3 nm. The implication is that the layers are of the order of 10 atomic layers thick. If the deposition of such films were done by atomic layer epitaxy (ALE) or other atomic layer deposition (ALD) techniques, the spectral results would fall in discrete patterns that could limit the potential design choices. The problem would be even more severe at shorter wavelengths. This work reports on the study of some of those possibilities and limitations.

## 1. INTRODUCTION

Interest in normal incidence mirrors at wavelengths of 12.4 nm and shorter has increased significantly in recent years. The thickness of a single atomic layer is on the order of 0.3 nm, depending on the material. The thickness of quarter wave optical thickness (QWOT) layers for 12.4 nm is approximately 10 times this thickness. If such layers were deposited by a process that retained an ordered crystalline structure, such as atomic layer epitaxy (ALE) or other atomic layer deposition (ALD) techniques, the layer thicknesses would be "quantized" to discrete thicknesses such as 9, 10, 11, etc. atomic layers thick. This ALE or ALD might have some advantages in thickness and scattering control, but would impose some constraints on what could be designed and the design techniques used.

The effects of dispersion will be ignored in this discussion for the sake of simplicity, even though the  $n$  and  $k$  values of real materials change rapidly with wavelength in the 12.4 nm spectral region. These illustrations will use Mo and Si as the two coating materials and glass as the substrate with the following indices: glass,  $N_G = 0.9813 + i0.0070$ ; Mo,  $N_{Mo} = 0.9324 + i0.0100$ ; Si,  $N_{Si} = 1.0319 + i0.0015$ . The atomic diameters, and thereby atomic layer thicknesses, of Mo and Si are taken as 0.278 and 0.264 nm respectively for the sake of this discussion.

## 2. EFFECTS OF ATOMIC LAYERS ON DESIGNS

Figure 1 shows an "amorphous" design for a 12.4 nm reflector where the layer thicknesses are not constrained to be an integral number of atomic layers. Also for simplicity, the design refinements of varying the ratio of the thickness of the Mo and Si layers as done by Yamamoto and Namioka<sup>1</sup> for optimum reflectance have not been used in this figure. The design is: (3.12Mo 3.26Si)48; forty-eight layer pairs of Mo and Si of 3.12 and 3.26 nm thickness respectively. Figure 2 shows a "quantized" design with its peak to the left, where the Mo layers are 11 atoms thick and the Si layers are 12 atoms thick, (3.058M 3.168S)48. The notation 11/12 will be used to designate such a design. The peak on the right of Fig. 2 is 12/12. This shows that the 11/12 and 12/12 designs would not provide optimum performance for the 12.4 nm reflector. The 12/11 design, which is not shown, gives a similar but not identical result to the 11/12 design.

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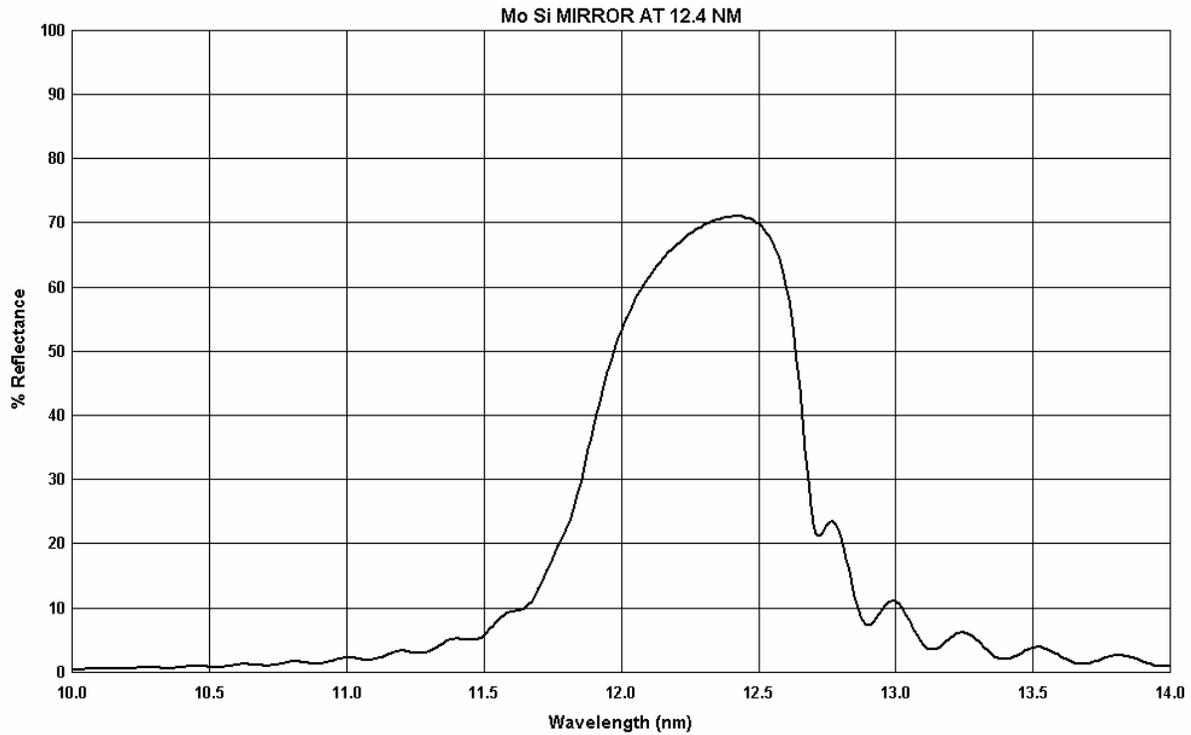


Figure 1: Amorphous design with no atomic layer thickness constraints. The design is: (3.058M 3.168S)48.

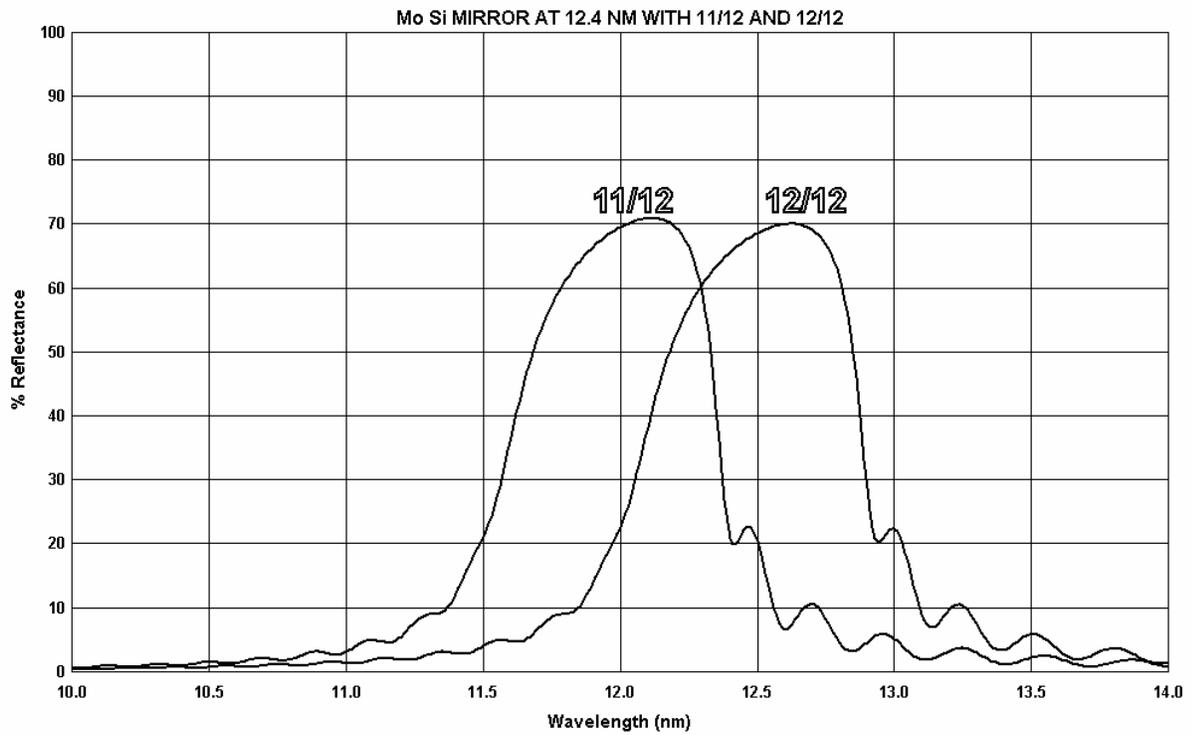
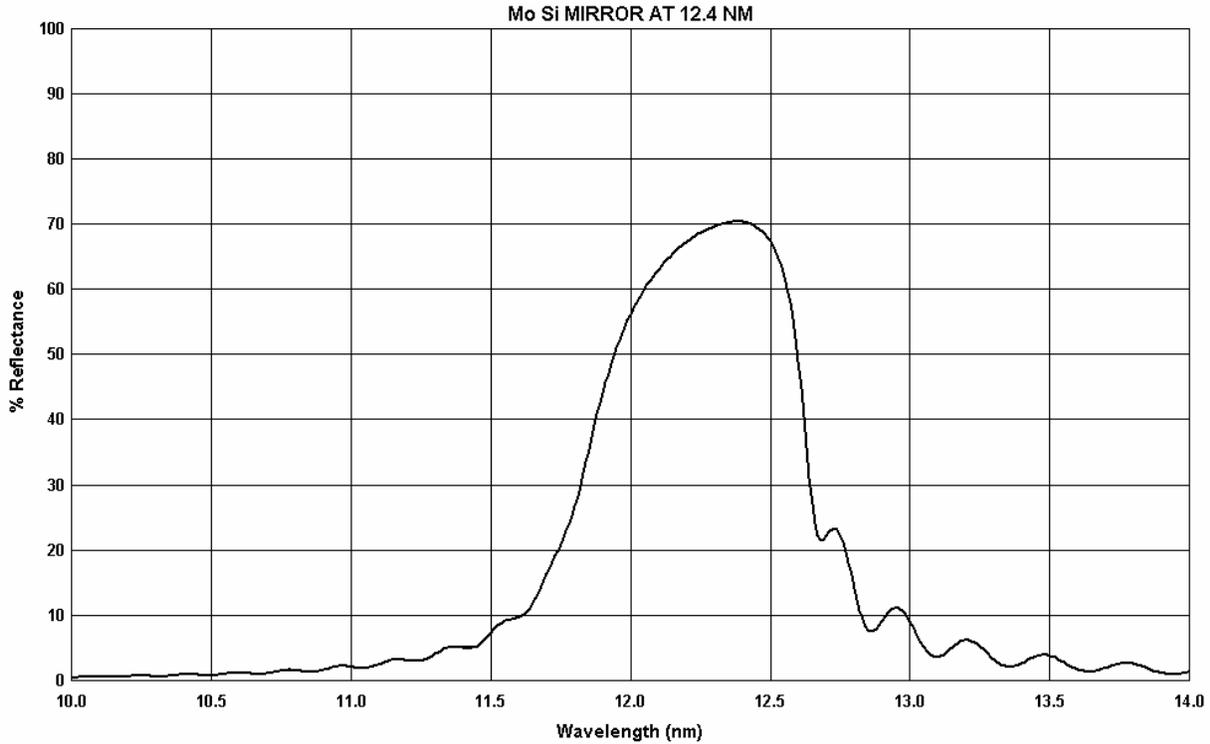


Figure 2: Quantized atomic layer thicknesses 11/12 (left) and 12/12 (right).

### 3. A METHOD TO OVERCOME THE LIMITATION

The fact that many layer pairs are needed to achieve high reflectance in these cases offers an opportunity to overcome the limitations described above. By interspersing layers of one more or one less atomic thickness in an otherwise regular stack of layer pairs, the designed reflectance peak can be shifted to longer or shorter wavelengths respectively. For example, by having half the layer pairs 11/12 and half 12/12, the resulting reflectance peak can be brought near to 12.4 as seen in Fig. 3. Such a design would be (3.058M 3.168S 3.336M 3.168S)24.



**Figure 3: Atomic layer design with half of the layer pairs at 11/12 interspersed with half at 12/12 pairs to shift the result to 12.4 nm peak wavelength. The design is: (3.058M 3.168S 3.336M 3.168S)24.**

If it were desired to shift the peak wavelength of the design to 12.5 nm as seen in Fig. 4, proportionately more 12/12 pairs would be used as in the following design: (3.058M 3.168S 3.336M 3.168S 3.336M 3.168S 3.336M 3.168S)12.

In Fig. 5, the higher peak is an amorphous design where the optimizing techniques of Yamamoto and Namioka<sup>1</sup> have been employed to get the "ideal" maximum reflectance which these materials can achieve at this wavelength. The lower curve was computed by taking the ideal design and rounding each layer thickness to the nearest integral atomic layer thickness. Figure 6 shows what these integer numbers would be for each layer of the ideal design if deposited this way. It can also be seen how the thickness of the Mo layers decreases as the outer surface layer is approached to satisfy the reflectance optimizing principles described by Yamamoto and Namioka<sup>1</sup> first generally described by Carniglia and Apfel<sup>2</sup>.

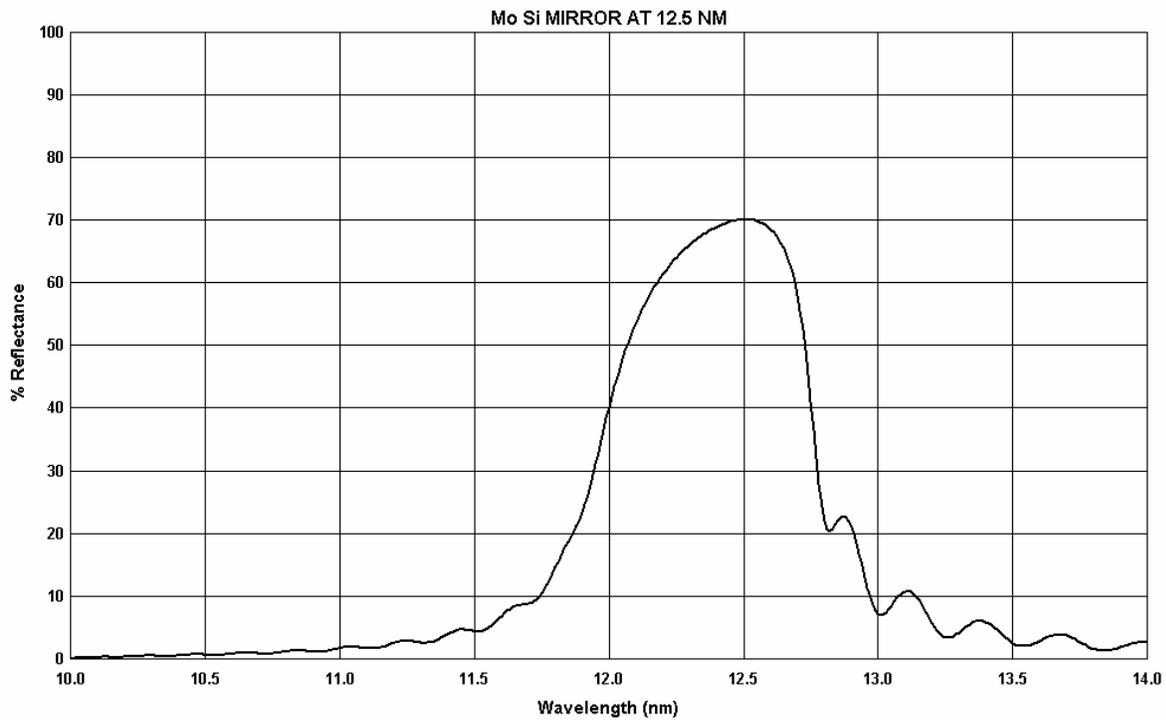


Figure 4: Atomic layer design with a greater portion of 12/12 pairs to shift the result to 12.5 nm peak wavelength. The design is: (3.058M 3.168S 3.336M 3.168S 3.336M 3.168S 3.336M 3.168S)12.

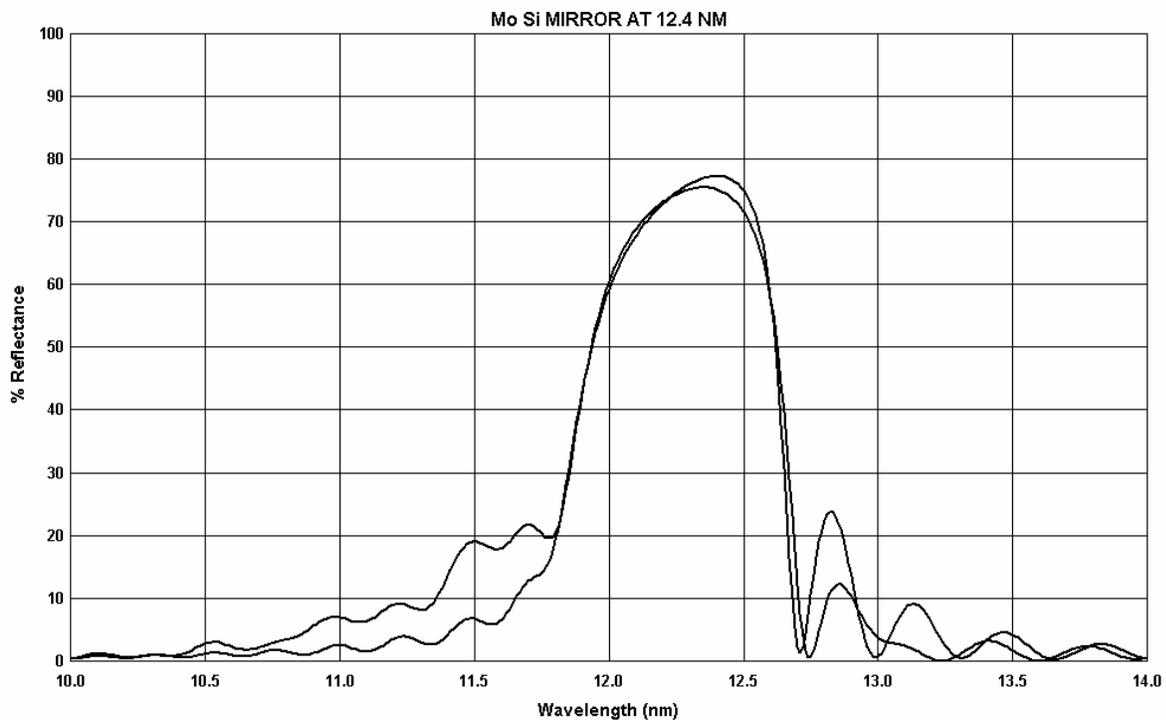
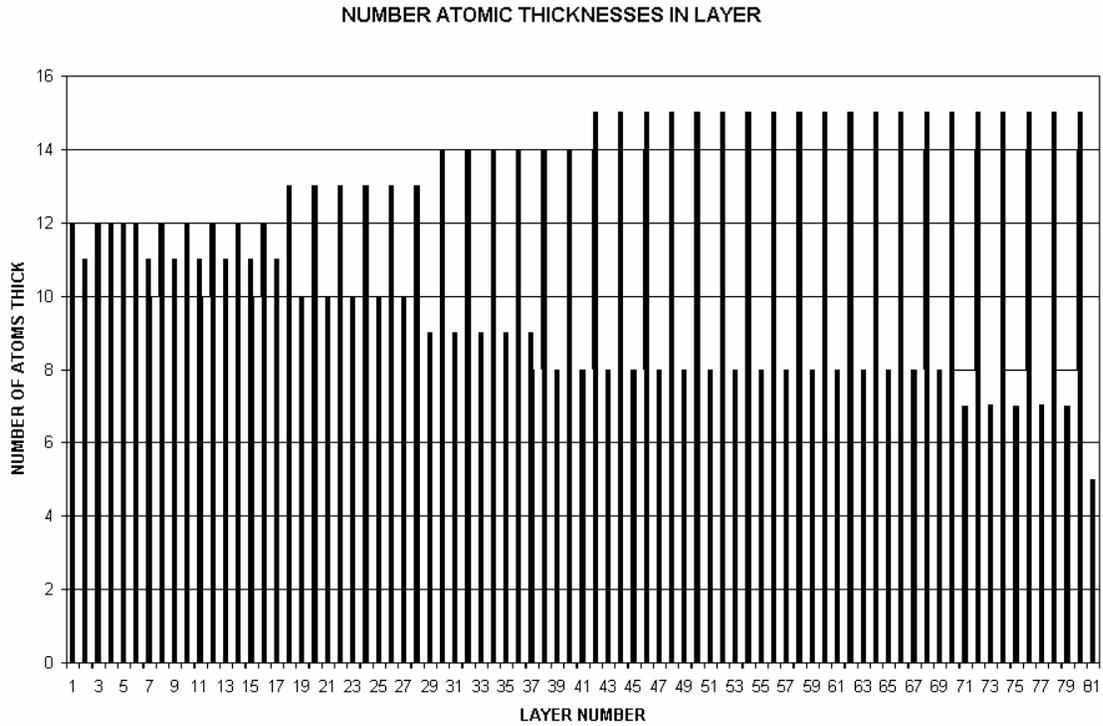
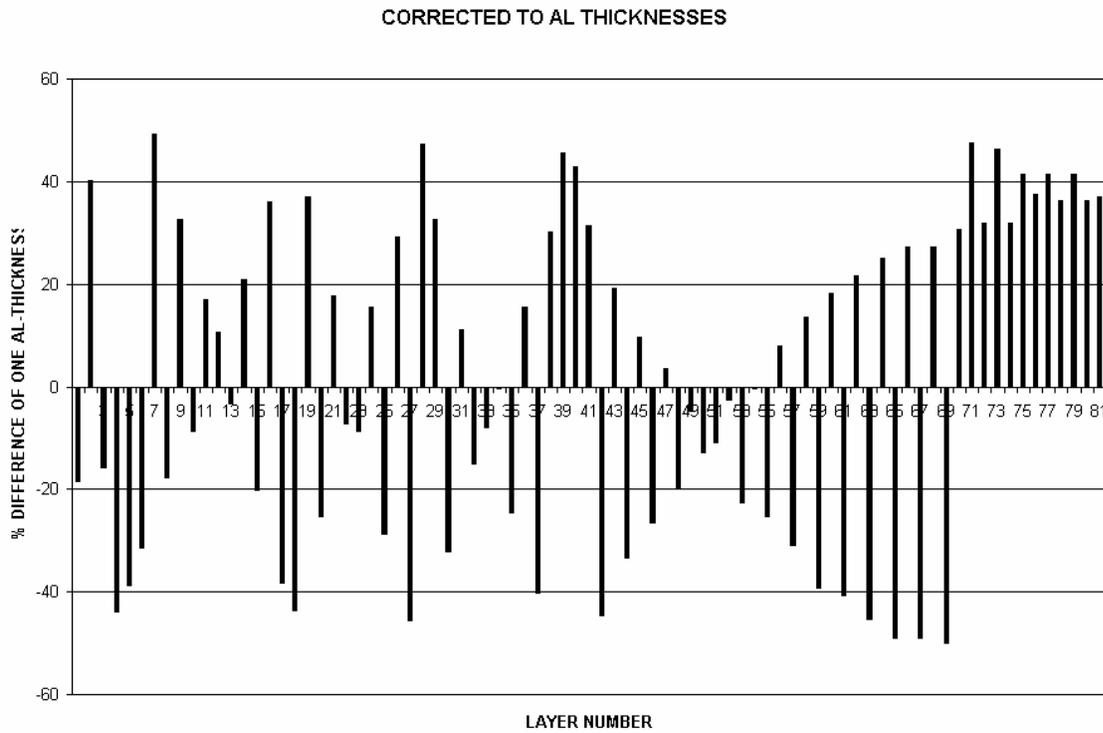


Figure 5: "Ideal" amorphous design (top) with atomic layer design (slightly lower).



**Figure 6:** Number of atomic layer thicknesses by layer number in the quantized design. Note that the more absorbing Mo layers get thinner with increasing layer number toward the outer layer in the vacuum.



**Figure 7:** Percent of an atomic thickness change to achieve an integral thickness for each layer.

Figure 7 shows how much each layer had to be changed (in percentage of an atomic layer (AL) thickness) from the ideal thickness to have an integral number of ALs. 50% one way or the other would be the maximum adjustment in thickness to reach the nearest intergral number of ALs.

Since the quantized result in Fig. 5 was short in wavelength by a small factor (and also short in reflectance), the starting ideal design was scaled by that small factor and then quantized again as before. Figure 8 shows a somewhat improved result over that of Fig. 5 as compared to the ideal amorphous design.

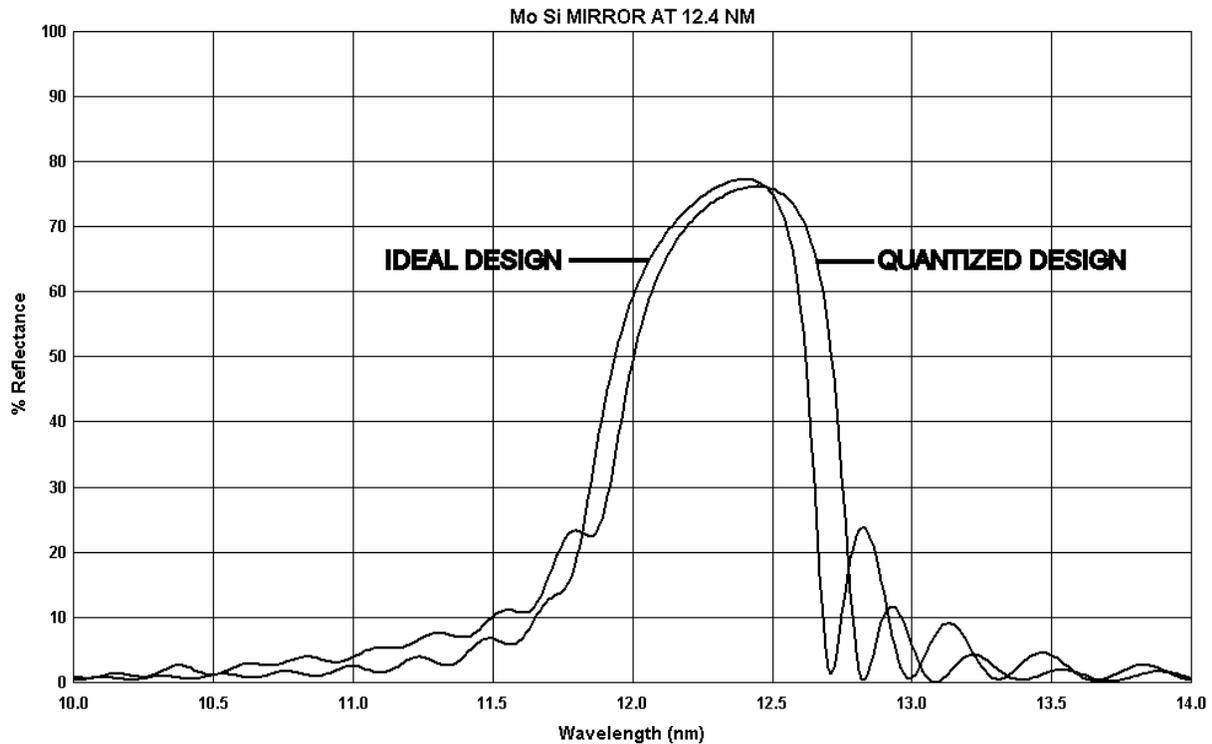


Figure 8: Ideal design shifted and then quantized again to achieve a wavelength change.

As another approach, the ideal design was attempted in quantized form by using the Southwell<sup>3</sup> "Flip-Flop Optimization" design technique as implemented in Goldstein's *Film-Star* software<sup>4</sup>. In this case, the high and low indices were taken for Mo and Si as given above, and the number of the individual (one atomic thickness) layers were taken as 940. The software changes each of these "atomic thickness layers" in sequence to determine which index gives the best result for that thin layer with respect to the design goal, 100% reflectance at 12.4 nm in this case. The design process iterates until no further progress is made. It is interesting to note in Fig. 9 that the Flip-Flop design using integral thickness atomic layers achieves almost the same result as the ideal design.

It is particularly interesting to note that the Flip-Flop technique arrived at a design from no *a priori* information or starting design, just the indices of refraction and the atomic layer thicknesses. However, Fig. 10 shows (in a somewhat different format from Fig. 6) that the same change in layer thicknesses with layer number has occurred with the Flip-Flop technique as with the method of Yamamoto and Namioka<sup>1</sup>. This would imply that the latter method is in accord with the natural solution to the problem, as seen by the fact that two radically different approaches yield the same result.

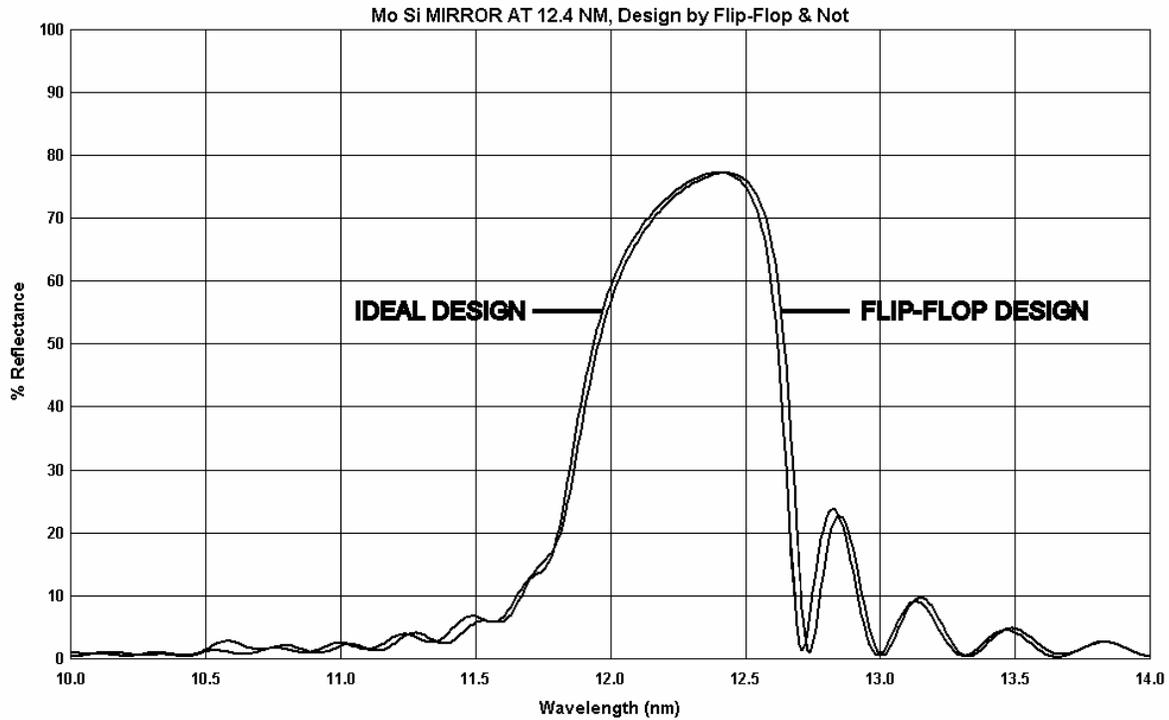


Figure 9: Ideal design compared to Flip-Flop optimized design with atomic layer thicknesses.

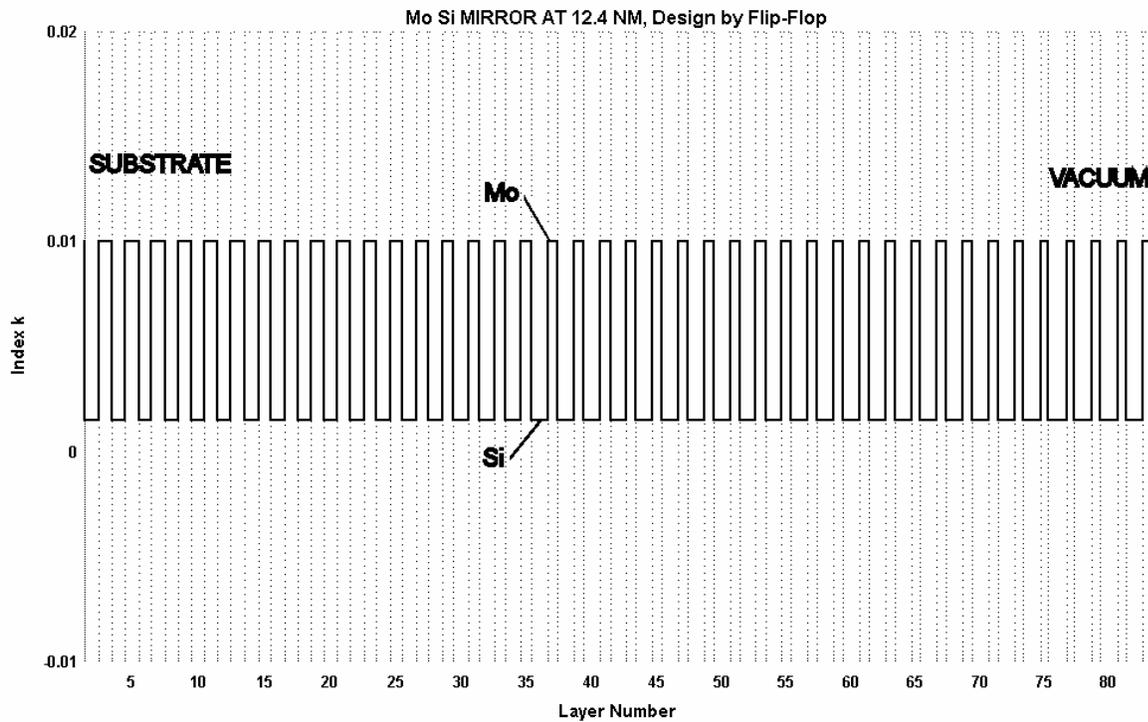


Figure 10: Index (k) values versus thickness for all layers. Note decreasing thickness of high index layers with layer number as in Fig. 6.

#### 4. CONCLUSIONS

It has been shown how the deposition of uniform atomic layers by ALE or ALD to form essentially crystalline structures would tend to "quantize" the wavelengths of the high reflection bands that could be achieved. However, techniques to overcome this limitation have been described wherein the thicknesses of the layers in the stack are varied and distributed within the quantized constraints of the individual layer thicknesses. It has been shown that the quantization effects of ALD or ALE are not a significant limitation at 12.4 nm when properly taken into account. However, at shorter wavelengths, it can be expected to become a proportionately greater problem. Some of the techniques described here may need to be employed to overcome those limitations.

#### REFERENCES

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