LASER INTERFEROMETER GRAVITATIONAL WAVE OBSERVATORY
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MASSACHUSETTS INSTITUTE OF TECHNOLOGY

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Analysis of DLC and Semiconductor AR Coatings for Stainless Steel Baffles

Michael Smith

LIGO Hanford Observatory
P.O. Box 1970; Mail Stop S9-02
Richland, WA 99352
Phone (509) 37208106
Fax (509) 372-8137
E-mail: info@ligo.caltech.edu

LIGO Livingston Observatory
19100 LIGO Lane
Livingston, LA 70754
Phone (225) 686-3100
Fax (225) 686-7189
E-mail: info@ligo.caltech.edu

California Institute of Technology
LIGO – MS 100-36
Pasadena, CA 91125
Phone (626) 395-2129
Fax (626) 304-9834
E-mail: info@ligo.caltech.edu

Massachusetts Institute of Technology
LIGO – MS NW22-295
Cambridge, MA 02139
Phone (617) 253-4824
Fax (617) 253-7014
E-mail: info@ligo.mit.edu

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1 INTRODUCTION

This document presents a theoretical analysis, based on Fresnel reflection theory, of the reflectance of polished stainless (SS) baffle surfaces with various proposed AR coatings. The analysis was compared with the measured reflectance values of a diamond-like-coating (DLC) applied to polished SS substrate obtained from R.Takahashi of KAGRA. The BRDF properties of DLC are similar to black glass.

A potential reduction in the scattered light displacement noise from baffles and beam dumps could be obtained by applying a suitable AR coating with low BRDF; e.g. an AR coating could be applied to the pre-fabricated polished SS surfaces of the Arm Cavity Baffle (ACB), in *lieu* of an oxidation coating.

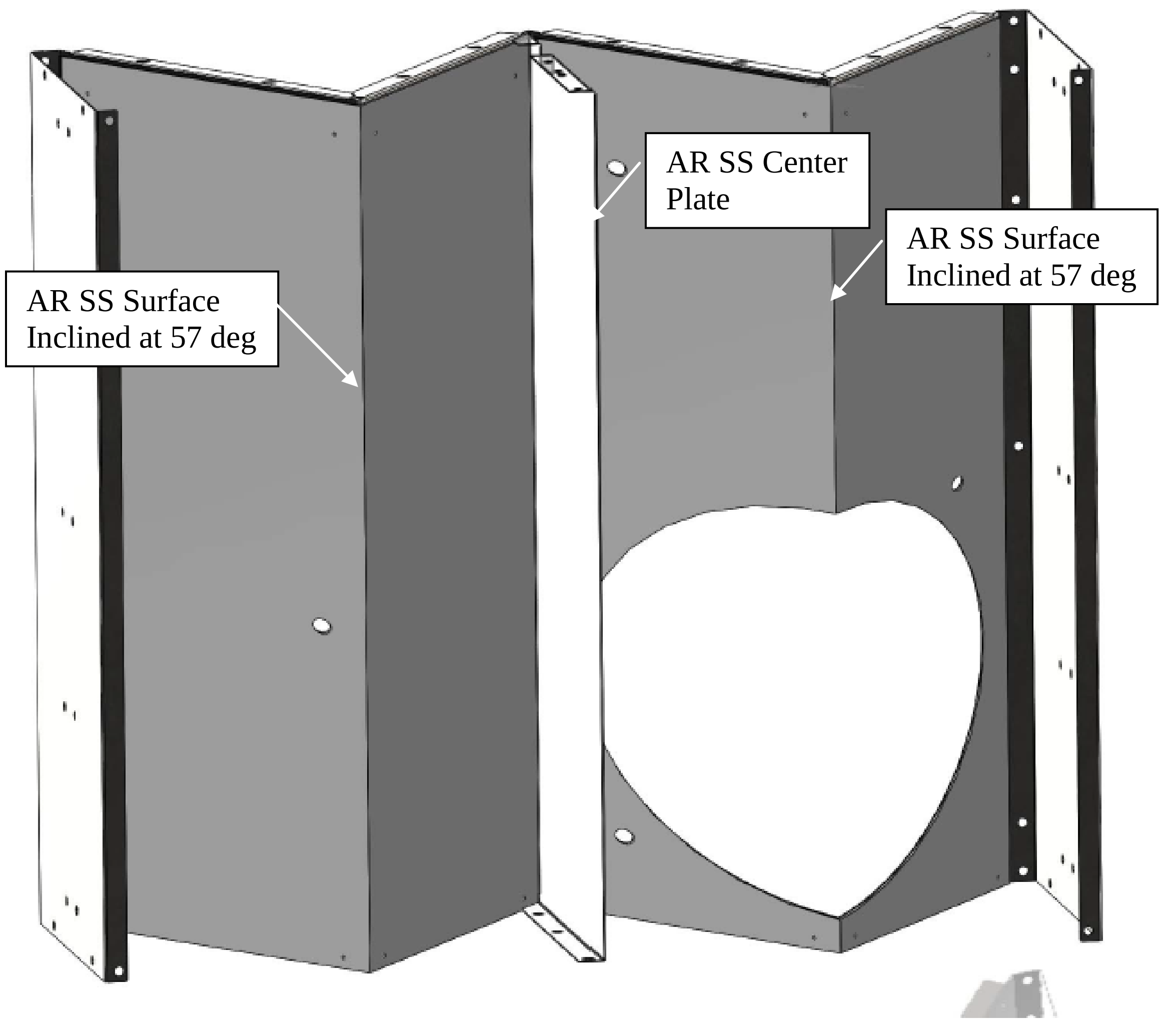

Figure 1: Arm Cavity Baffle with AR Coated SS

With the "V" shaped design of the aLIGO baffles, the displacement noise from back-scattered light by the baffle can be minimized by reducing the BRDF and the reflectivity of the baffle surfaces at 57 deg incidence angle

2 REFERENCES

1. Pedrotti & Pedrotti, Introduction to Optics, 2^{nd} Ed. Prentice Hall, New Jersey (1993)
2. R. Takahashi et al. Vacuum 73 (2004) 145-148
3. Useful index of refraction data can be found at RefractiveIndex.INFO

3 FRESNEL REFLECTION ANALYSIS

A thin film with index n2 and thickness h is coated onto a metal substrate of index n3 and immersed in vacuum (or air) with index n1, as shown schematically in Figure 2.

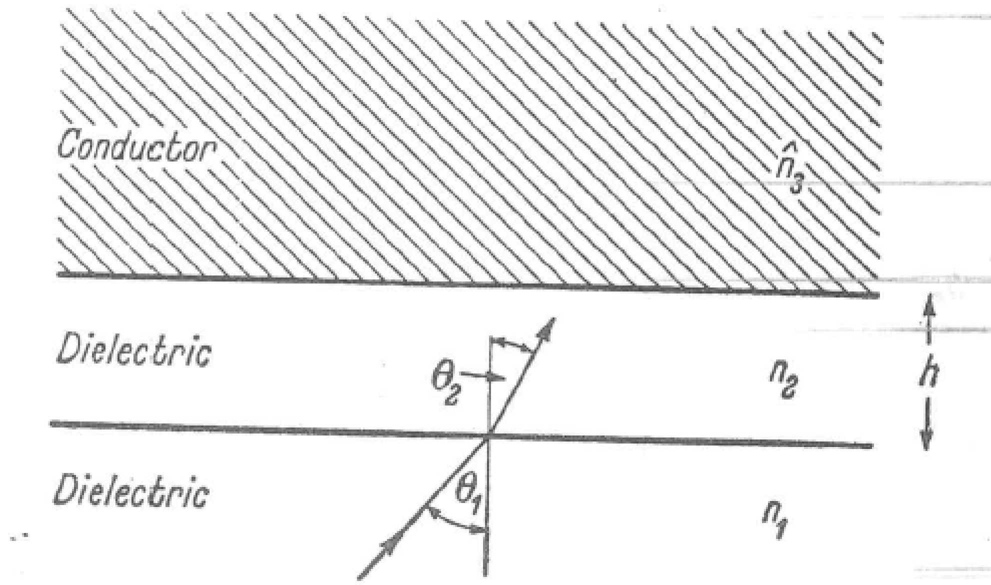

Figure 2: Geometry for Fresnel Reflection Analysis

The incident light field can be either TM p-polarization or TE s-polarization. The transmitted field through surface 1-2 reflects from the metal surface 2-3 and then transmits internally through surface 2-1; the reflected field from surface 2-3 will also undergo an internal reflection from surface 2-1, followed by a subsequent reflection from surface 2-3 and internal transmission through surface 2-1. The internally reflected fields within the AR coating travel through varying optical thicknesses depending upon the number of internal reflections, which cause the emerging fields at the outer surface of the AR coated SS to have varying phase retardation and varying amplitudes due to the index of refraction and absorptivity within the AR coating.

The emerging fan of waves from multiple internal reflections between the two surfaces bounding the AR coating will recombine with the first surface external reflection from surface 1-2 and reduce the intensity of the reflected field.

3.1 Parameters

vacuum wavelength, m $\lambda_0 := 1.064 \cdot 10^{-6}$

index of vacuum $n_1 := 1$

index of SS substrate $n_{ss} := 2.5 + 4.1i$

$n_3 := n_{ss}$

index of DLC AR coating $n_{dlc} := 2.4 + 0.04i$

index of AR coating $n_2 := n_{dlc}$

power absorption coefficient, m^-1 $\alpha(n_2) := \frac{4 \cdot \pi}{\lambda_0} \cdot |\mathrm{Im}(n_2)|$

relative index of AR coating, external $n_{2R}(n_2) := \frac{n_2}{n_1}$

relative index of SS substrate $n_{3R}(n_2, n_3) := \frac{n_3}{n_2}$

index of InSb AR coating $n_{insb} := 4.2 + 0.325i$

index of AlInP AR coating $n_{alinp} := 2.7 + 0.073i$

index of CdZnTe AR coating $n_{cdznte} := 2.8 + 0.031i$

incidence angle, rad $\theta_1 := 57 \cdot \frac{\pi}{180}$

incidence angle, deg $\theta_{1deg}(\theta_1) := \theta_1 \cdot \frac{180}{\pi}$

angle inside AR coating, rad

$$\theta_2(\theta_1, n_1, n_2) := \operatorname{asin}\left(\frac{n_1}{n_2}\cdot\sin(\theta_1)\right)$$

$$\theta_2(\theta_1, n_1, n_2) = 0.357 - 6.214i \times 10^{-3}$$

angle inside SS, rad

$$\theta_3(\theta_1, n_1, n_2, n_3) := \operatorname{asin}\left(\frac{n_2}{n_3}\cdot\sin(\theta_2(\theta_1, n_1, n_2))\right)$$

$$\theta_3(\theta_1, n_1, n_2, n_3) = 0.09 - 0.149i$$

3.2 Reflection from Uncoated SS Surface, P-Polarization

According to Pedrotti & Pedrotti, the Fresnel equations are valid with the complex indexes of refraction of the AR coatings and the SS substrate. This results in complex angles and complex reflection coefficients. The imaginary coefficients imply absorption of the fields and phase shifts due to polarization changes within the materials.

external reflection coefficient for SS surface

$$r_{1Pp}(\theta_1, n_{ss}) := \frac{n_{2R}(n_{ss})^2\cdot\cos(\theta_1) - \sqrt{n_{2R}(n_{ss})^2 - \sin(\theta_1)^2}}{n_{2R}(n_{ss})^2\cdot\cos(\theta_1) + \sqrt{n_{2R}(n_{ss})^2 - \sin(\theta_1)^2}}$$

$$r_{1Pp}(\theta_1, n_2) = 0.165 + 6.979i \times 10^{-3}$$

Reflectance from uncoated SS surface

$$R_{ssPp}(\theta_1, n_{ss}) := \left|r_{1Pp}(\theta_1, n_{ss})^2\right|$$

$$R_{ssPp}(\theta_1, n_{ss}) = 0.474$$

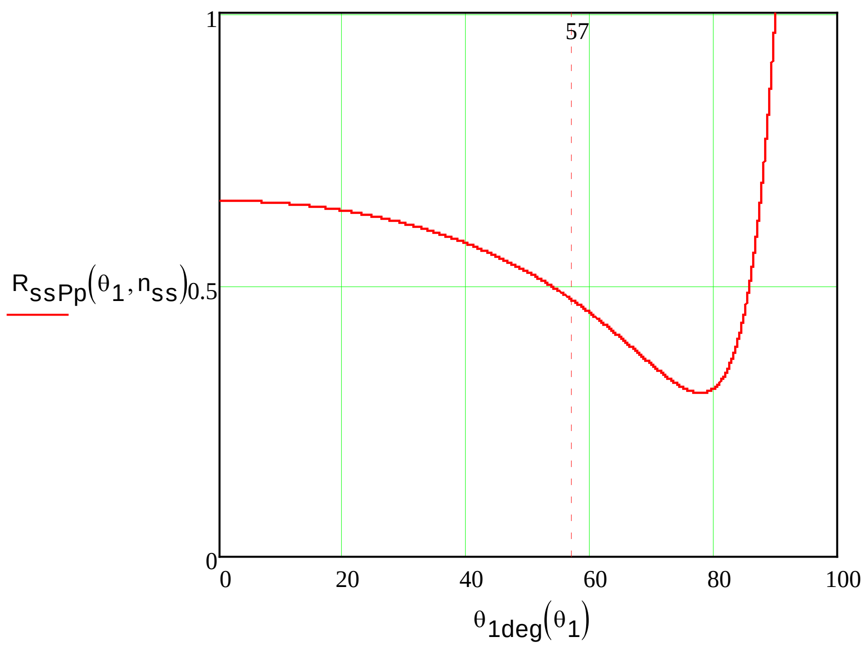

Figure 3: Reflectance from Uncoated Polished SS Surface, p-Polarization

3.3 AR Coating on SS, P-Polarization (TM Field)

reflection coefficient for surface 1-2

$$r_{1Pp}(\theta_1, n_2) := \frac{n_{2R}(n_2)^2 \cdot \cos(\theta_1) - \sqrt{n_{2R}(n_2)^2 - \sin(\theta_1)^2}}{n_{2R}(n_2)^2 \cdot \cos(\theta_1) + \sqrt{n_{2R}(n_2)^2 - \sin(\theta_1)^2}}$$

$$r_{1Pp}(\theta_1, n_2) = 0.312 + 6.939i \times 10^{-3}$$

reflection coefficient for surface 2-3

$$r_{2Pp}(\theta_1, n_1, n_2, n_3) := \frac{n_{3R}(n_2, n_3)^2 \cdot \cos(\theta_2(\theta_1, n_1, n_2)) - \sqrt{n_{3R}(n_2, n_3)^2 - \sin(\theta_2(\theta_1, n_1, n_2))^2}}{n_{3R}(n_2, n_3)^2 \cdot \cos(\theta_2(\theta_1, n_1, n_2)) + \sqrt{n_{3R}(n_2, n_3)^2 - \sin(\theta_2(\theta_1, n_1, n_2))^2}}$$

$$r_{2Pp}(\theta_1, n_1, n_2, n_3) = 0.397 + 0.478i$$

additional round trip phase difference between first surface reflection and internally reflected beam, rad

introduce the power absorption coefficient

$$\alpha(n_2) := \frac{4 \cdot \pi}{\lambda_0} \cdot |\mathrm{Im}(n_2)|$$

$$\delta_P(\theta_1, n_1, n_2, h) := \frac{4 \cdot \pi}{\lambda_0} \cdot \mathrm{Re}(n_2) \cdot \cos(\theta_2(\theta_1, n_1, n_2)) \cdot h + i \cdot \alpha(n_1) \cdot (\cos(\theta_2(\theta_1, n_1, n_2)) \cdot h)$$

$$\delta_P(\theta_1, n_1, n_2, h) = 27.743 + 0.036i$$

The infinite sum of internally reflected fields can be written in a closed form using Airy's equations.

effective reflection coefficient for surface 1-2 with infinite sum of multiple internal reflections

$$r_{1Ppeff}(\theta_1, n_1, n_2, n_3, h) := \frac{r_{1Pp}(\theta_1, n_2) + r_{2Pp}(\theta_1, n_1, n_2, n_3)\cdot e^{i\cdot\frac{4\cdot\pi}{\lambda_0}\cdot \mathrm{Re}(n_2)\cdot\cos(\theta_2(\theta_1, n_1, n_2))\cdot h}\cdot e^{-\alpha(n_2)\cdot\cos(\theta_2(\theta_1, n_1, n_2))\cdot h}}{1 + r_{1Pp}(\theta_1, n_2)\cdot r_{2Pp}(\theta_1, n_1, n_2, n_3)\cdot e^{i\cdot\frac{4\cdot\pi}{\lambda_0}\cdot \mathrm{Re}(n_2)\cdot\cos(\theta_2(\theta_1, n_1, n_2))\cdot h}\cdot e^{-\alpha(n_2)\cdot\cos(\theta_2(\theta_1, n_1, n_2))\cdot h}}$$

$$r_{1Ppeff}(\theta_1, n_1, n_2, n_3, h) = -0.042 - 0.138i$$

effective reflectance of AR coated SS

$$R_{1Ppeff}(\theta_1, n_1, n_2, n_3, h) := \left|\left(r_{1Ppeff}(\theta_1, n_1, n_2, n_3, h)\right)^2\right|$$

$$R_{1Ppeff}(\theta_1, n_1, n_2, n_3, h) = 0.021$$

4 TAKAHASHI DLC COATING ON SS

A DLC AR coating on SS was obtained from R. Takahashi of the KAGRA group. The properties of this coating were previously reported by R. Takahashi et al. The film was deposited using direct current plasma chemical vapor deposition (CVD), 120 mA @ 500V.

The sample's reflectivity and BRDF versus angle were subsequently measured at Caltech.

The first column of the matrix Rdlc is a list of incident angles in radians; the second column is the measured optical power reflectance; and the third column is the theoretical optical power reflectance for p-polarized light derived previously.

4.1 Reflectivity Data

Reflectivity of DLC Coating on SS, P-pol

$$R_{dlc} := \begin{pmatrix} 5\cdot\frac{\pi}{180} & 0.0048 & R_{1Ppeff}\left(5\cdot\frac{\pi}{180}, n_1, n_2, n_3, h\right) \\ 10\cdot\frac{\pi}{180} & 0.0053 & R_{1Ppeff}\left(10\cdot\frac{\pi}{180}, n_1, n_2, n_3, h\right) \\ 15\cdot\frac{\pi}{180} & 0.008 & R_{1Ppeff}\left(15\cdot\frac{\pi}{180}, n_1, n_2, n_3, h\right) \\ 20\cdot\frac{\pi}{180} & .0127 & R_{1Ppeff}\left(20\cdot\frac{\pi}{180}, n_1, n_2, n_3, h\right) \\ 30\cdot\frac{\pi}{180} & 0.037 & R_{1Ppeff}\left(30\cdot\frac{\pi}{180}, n_1, n_2, n_3, h\right) \\ 40\cdot\frac{\pi}{180} & 0.066 & R_{1Ppeff}\left(40\cdot\frac{\pi}{180}, n_1, n_2, n_3, h\right) \\ 50\cdot\frac{\pi}{180} & 0.11 & R_{1Ppeff}\left(50\cdot\frac{\pi}{180}, n_1, n_2, n_3, h\right) \\ 57\cdot\frac{\pi}{180} & 0.11 & R_{1Ppeff}\left(57\cdot\frac{\pi}{180}, n_1, n_2, n_3, h\right) \\ 60\cdot\frac{\pi}{180} & 0.13 & R_{1Ppeff}\left(60\cdot\frac{\pi}{180}, n_1, n_2, n_3, h\right) \\ 70\cdot\frac{\pi}{180} & 0.16 & R_{1Ppeff}\left(70\cdot\frac{\pi}{180}, n_1, n_2, n_3, h\right) \\ 80\cdot\frac{\pi}{180} & 0.31 & R_{1Ppeff}\left(80\cdot\frac{\pi}{180}, n_1, n_2, n_3, h\right) \end{pmatrix}$$

A least squares analysis was performed to determine the best thickness value, h, that matches all the data points.

The following complex index of refraction values presented in the Takahashi paper were used for the calculation.

$n_1 := 2.4 + 0.04i$

$n_2 := 2.5 + 4.1i$

Note, that Takahashi uses the complex conjugate for the imaginary part of the index, whereas in this document the convention of Pedrotti is used with a positive value for the imaginary index.

The best-fit thickness for the sample film thickness is d = 0.974 E-6 m. The calculated reflectance curve is compared with the experimental data in Figure 4.

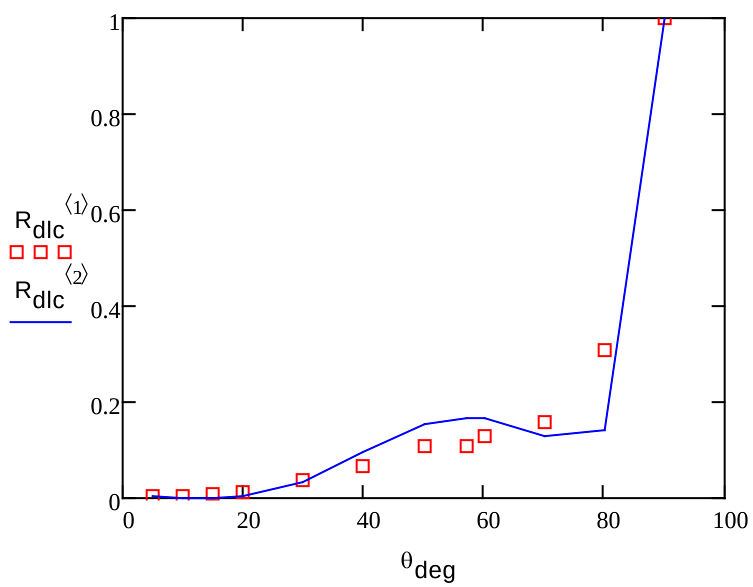

Figure 4: Theoretical Reflectance, p-polarization, Compared with Takahashi DLC Sample Data—Best-fit Thickness d = 0.974 E-6 m.

The experimental reflectance data presented by Takahashi et al in their paper show a pronounced dip in reflectance at approximately 40 deg incidence angle—the dip was not seen in the sample tested at Caltech, and they state a best-fit thickness of d = 1.016 E-6 m for p-polarization. This discrepancy between their report and the sample tested at Caltech could be explained if the samples were from different coating runs, or from a different placement within the coating chamber, thereby resulting in slightly different thicknesses.

4.2 DLC and Black Glass BRDF Data

The back-scatter BRDF of the Takahashi DLC coating on SS @ 57 degrees incidence angle was measured at Caltech by Smith to be 8E-5 sr^-1, as shown in Figure 5. The BRDF of DLC is comparable to the measured value of black glass, 4E-5 sr^-1, as shown in Figure 6.

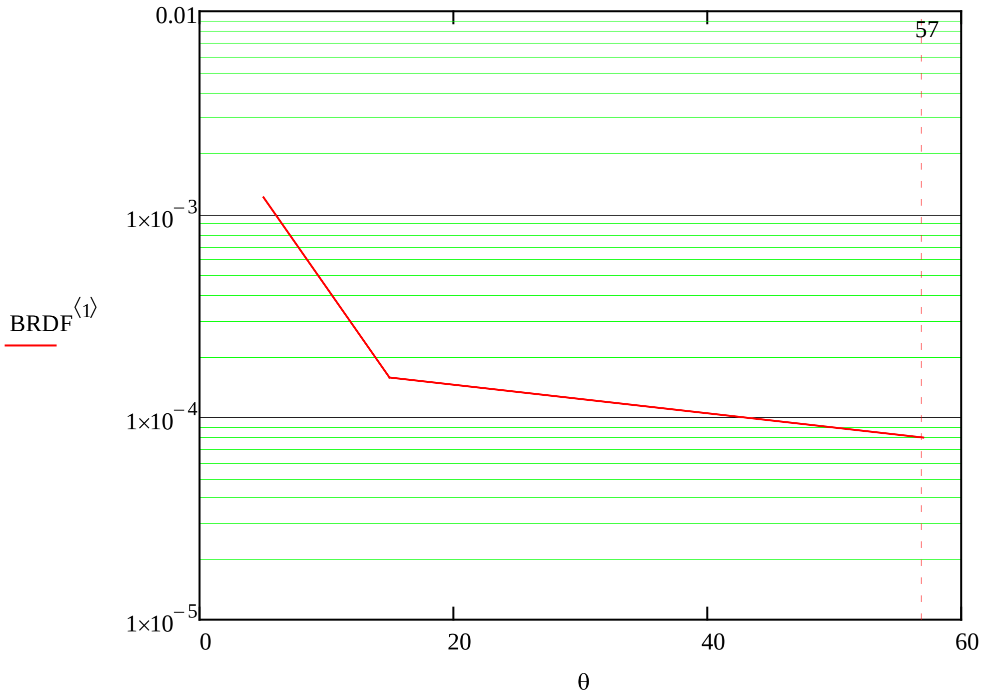

Figure 5: Back-Scatter BRDF Sr^-1 of DLC Coating on SS, vs Incidence Angle

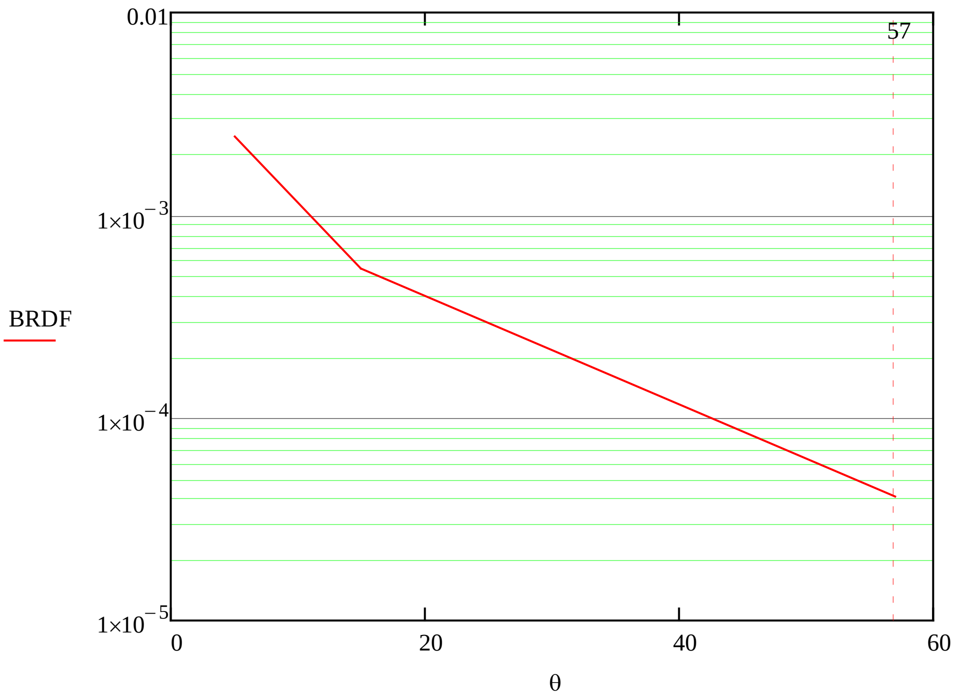

Figure 6: Back-Scatter BRDF of Black Glass Sr^-1, vs Incidence Angle

5 DLC AR COATING ON SS, OPTIMIZED FOR 57 DEG INCIDENCE ANGLE

The calculated reflectance from a DLC-coated SS substrate oscillates through maxima and minima with increasing film thickness because of the periodic phase difference caused by the optical distance traveled through the AR film. In addition, the minimum reflectance becomes progressively smaller with increasing film thickness because of the absorption within the DLC film, and reaches a minimum value as shown in Figure 7.

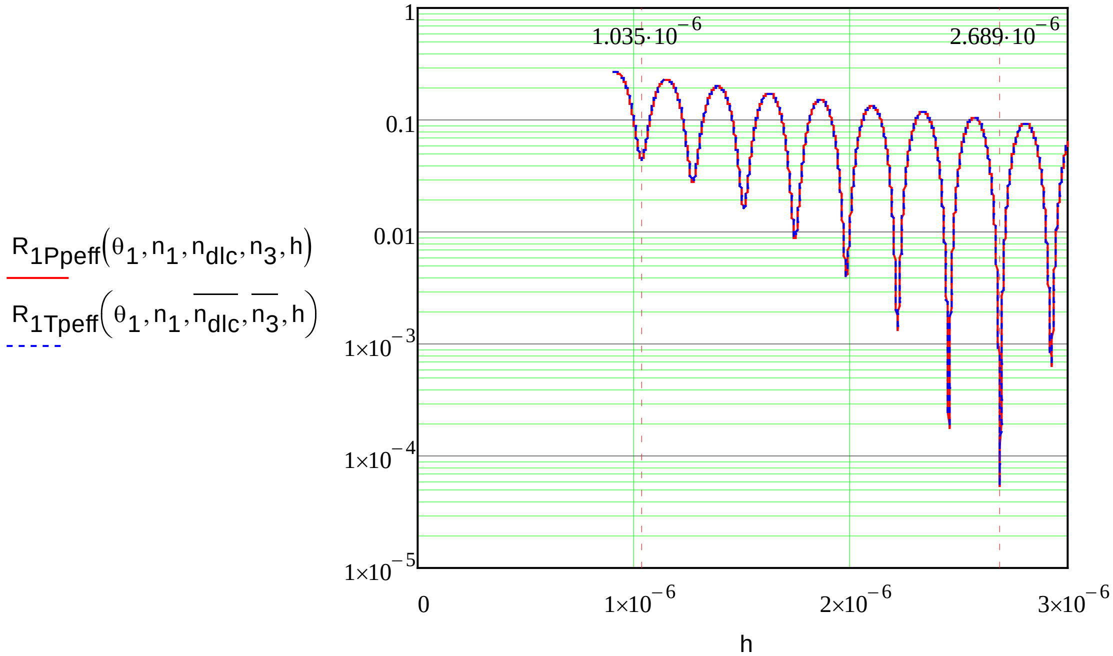

Figure 7: Reflectance of DLC AR Coating on SS vs Coating Thickness

The optimum thickness of the DLC AR coating for minimum reflectance at 57 deg incidence angle appears to be 2.689E-6 m.

The reflectance of the DLC-coated SS as a function of incidence angle with two different coating thicknesses is shown in Figure 8.

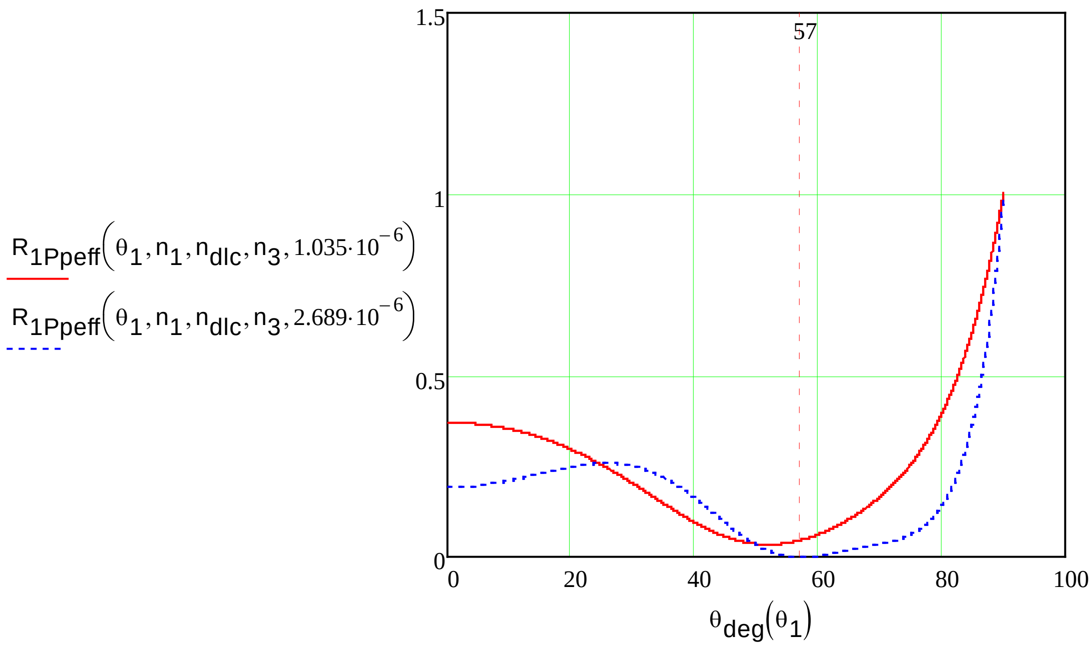

Figure 8: Calculated Reflectance of DLC AR Coating on SS vs Incident Angle

6 SEMICONDUCTOR AR COATINGS ON SS

The most suitable material for AR coating on SS should have a real index of refraction approximately the same magnitude as the real index of SS, and an imaginary index—extinction coefficient—approximately 0.1 to 0.01 times smaller, as is the case for DLC.

index of SS substrate $n_{ss} := 2.5 + 4.1i$

index of DLC AR coating $n_{dlc} := 2.4 + 0.04i$

This combination of real and imaginary terms keeps the maximum oscillatory reflectance from being too large, and results in minimum reflectivity for a film of approximately 1E-6 m thickness.
DLC, AlInP, and CdZnTe appear to be suitable materials for AR coating on SS.
Of course, another important characteristic of the AR coating is that the deposited film should be extremely dense with a low surface scatter; low scattering can be enhanced by using ion beam deposition techniques for materials that are supplied in bulk form.

6.1 INSB AR COATING ON SS, OPTIMIZED FOR 57 DEG INCIDENCE ANGLE

The calculated reflectance from an InSb-coated SS substrate, optimized for 57 deg incidence angle, is shown in Figure 9.

index of InSb $n_{insb} = 4.2 + 0.325i$

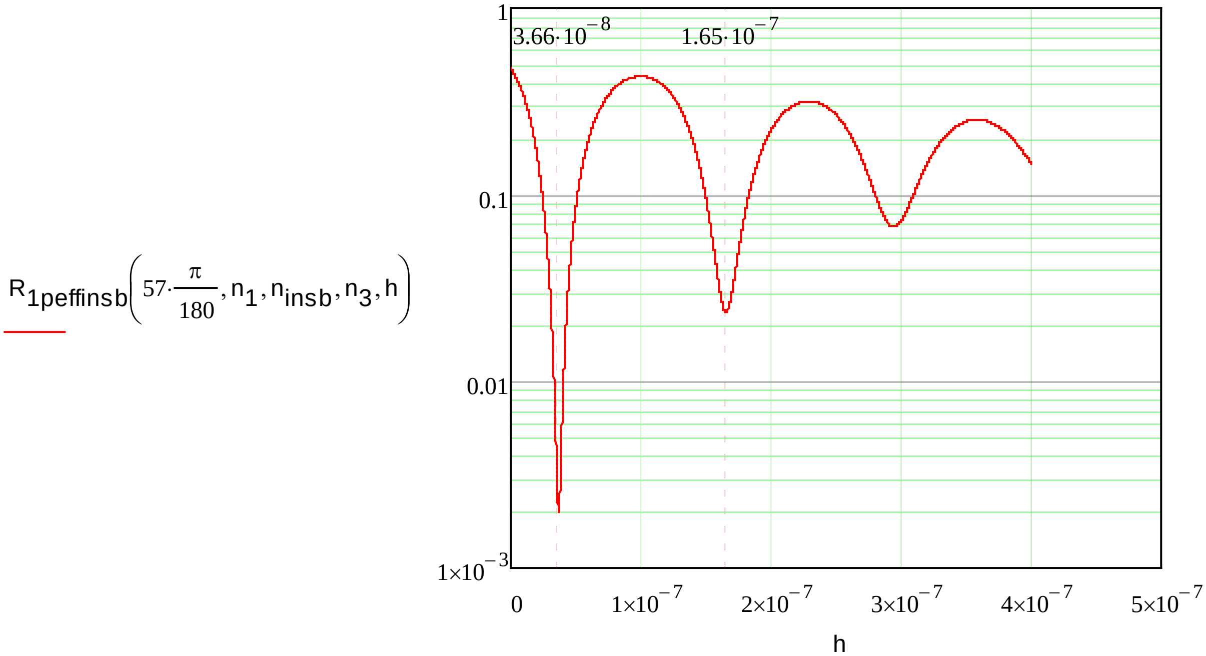

Figure 9: Calculated Reflectance of InSb AR Coating on SS vs Coating Thickness

The optimum thickness of the InSb film for minimum reflectance at 57 deg incidence angle appears to be 3.66E-8 m. However, a more practical thickness would be the second minimum at a thickness of 1.65E-7.
The calculated reflectance of InSb-coated SS as a function of incidence angle for the two thicknesses is shown in Figure 10.

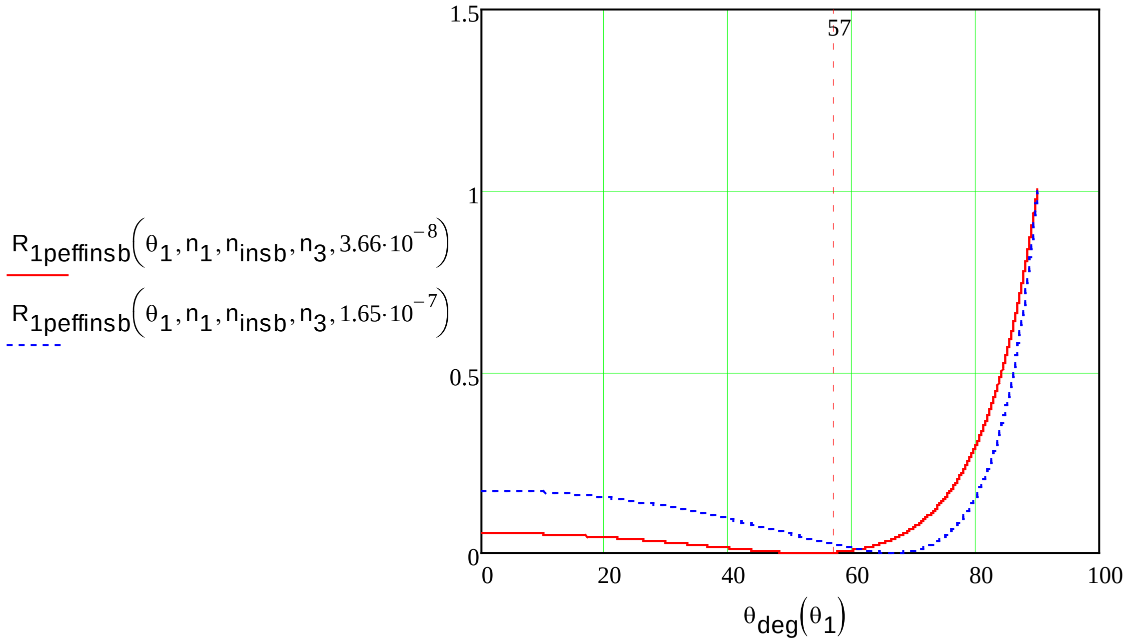

Figure 10: Calculated Reflectance of InSb AR Coating on SS vs Incident Angle

6.2 ALINP AR COATING ON SS, OPTIMIZED FOR 57 DEG INCIDENCE ANGLE

The calculated reflectance from an AlInP-coated SS substrate, optimized for 57 deg incidence angle, is shown in Figure 11.

index of AlInP $n_{alinp} = 2.7 + 0.073i$

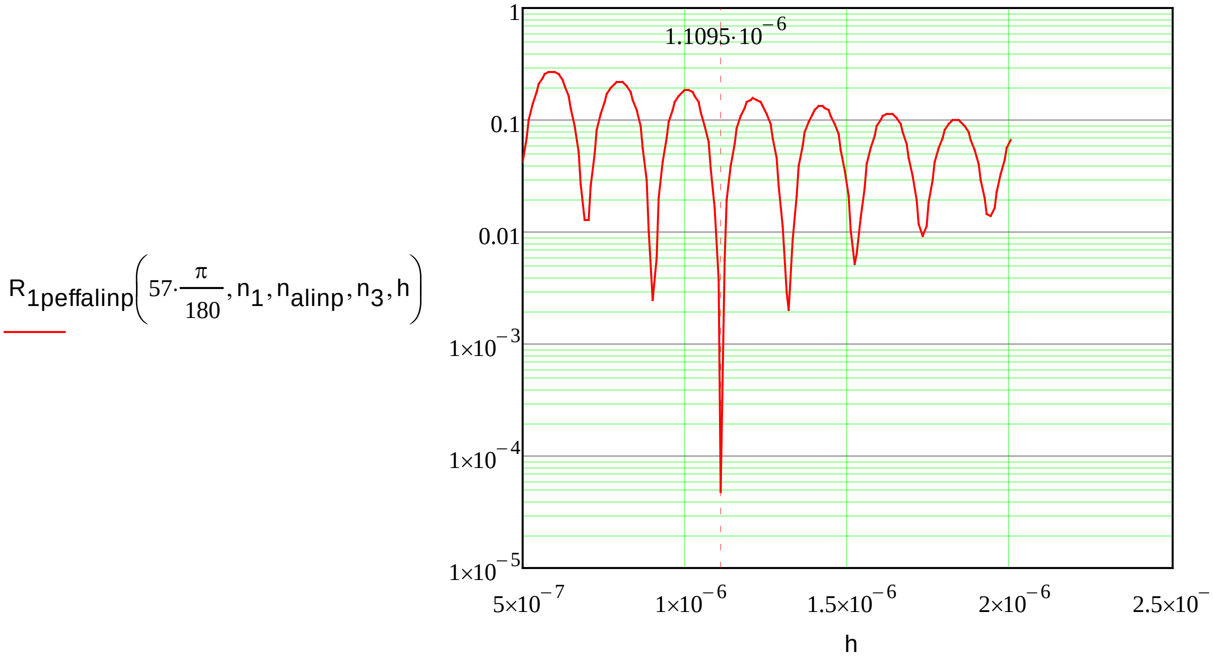

Figure 11: Calculated Reflectance of AlInP AR Coating on SS vs Coating Thickness

The optimum thickness of the AlInP coating for minimum reflectance at 57 deg incidence angle appears to be 1.1095E-6 m.
The calculated reflectance of AlInP -coated SS as a function of incidence angle is shown in Figure 12.

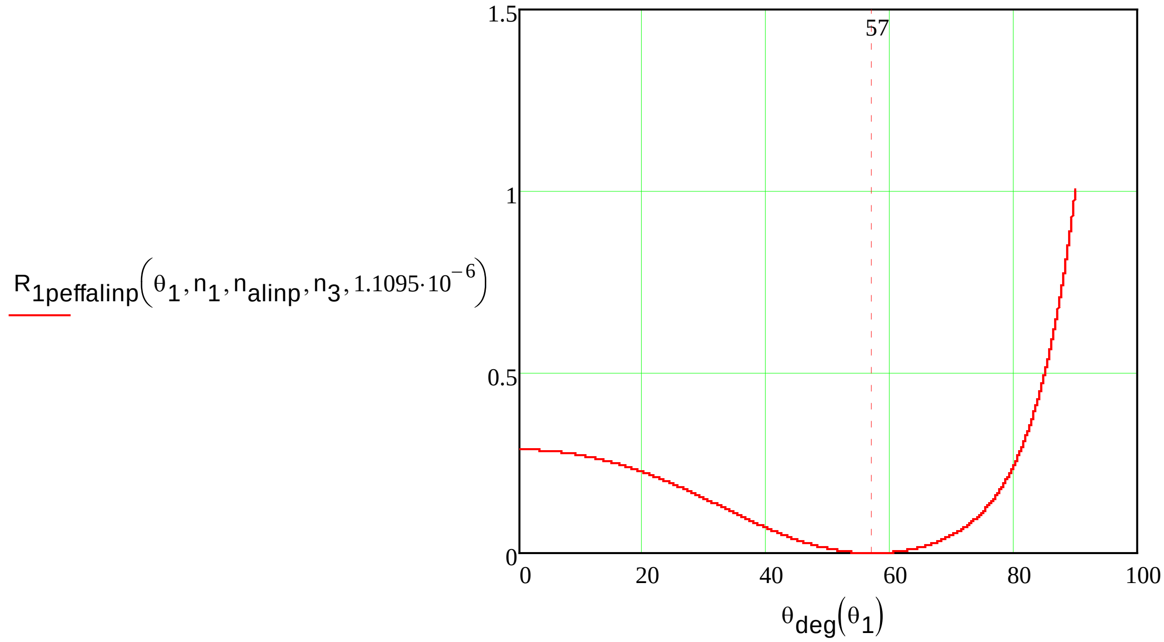

Figure 12: Calculated Reflectance of AlInP AR Coating on SS vs Incident Angle

6.3 CDZNTE AR COATING ON SS, OPTIMIZED FOR 57 DEG INCIDENCE ANGLE

The calculated reflectance from a CdZnTe-coated SS substrate vs thickness, optimized for 57 deg incidence angle, is shown in Figure 13.

index of CdZnTe $n_{cdznte} = 2.8 + 0.031i$

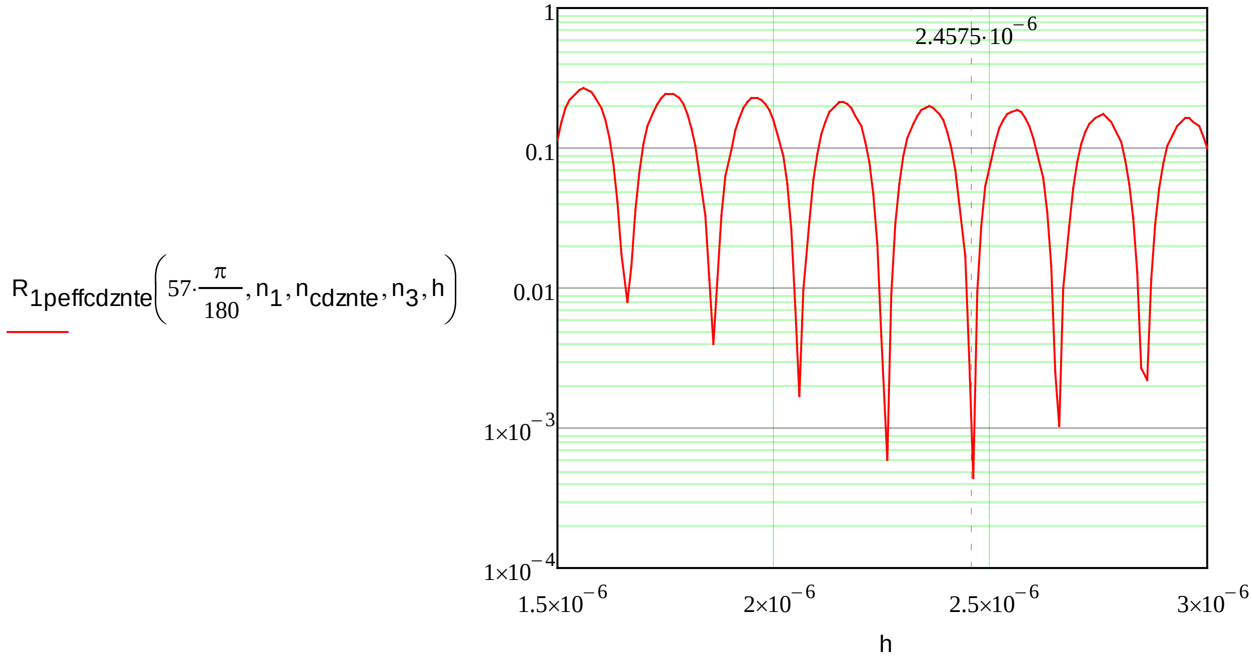

Figure 13: Calculated Reflectance of CdZnTe AR Coating on SS vs Coating Thickness

The optimum thickness of the CdZnTe coating for minimum reflectance at 57 deg incidence angle appears to be 2.458E-6 m.
The calculated reflectance of CdZnTe-coated SS as a function of incidence angle is shown in Figure 14.

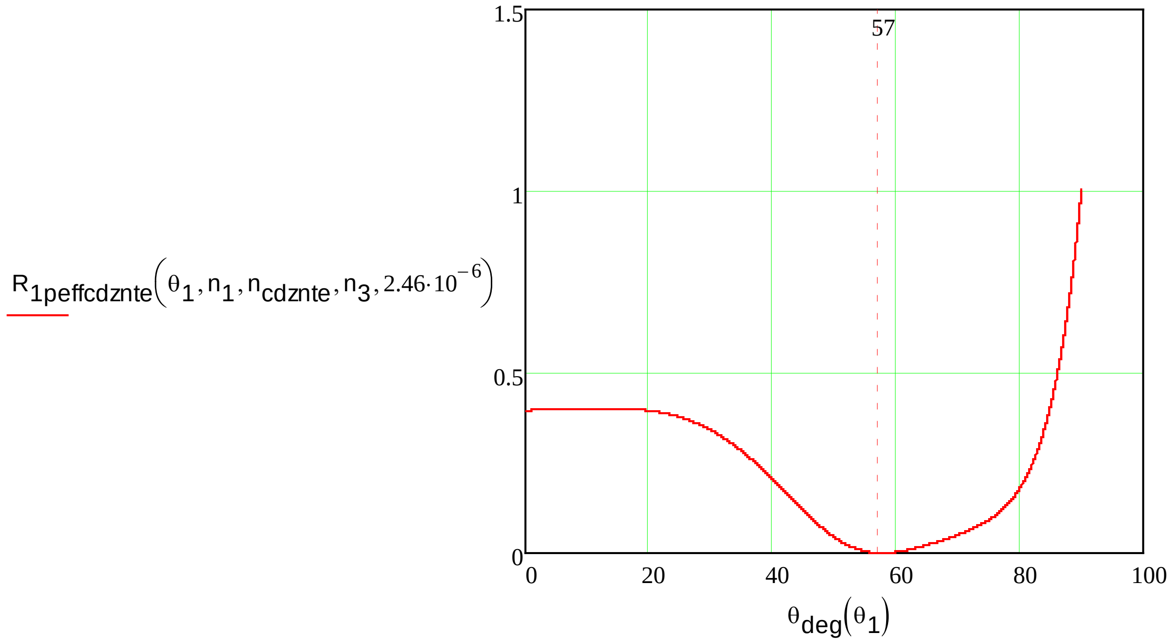

Figure 14: Calculated Reflectance of CdZnTe AR Coating on SS vs Incident Angle