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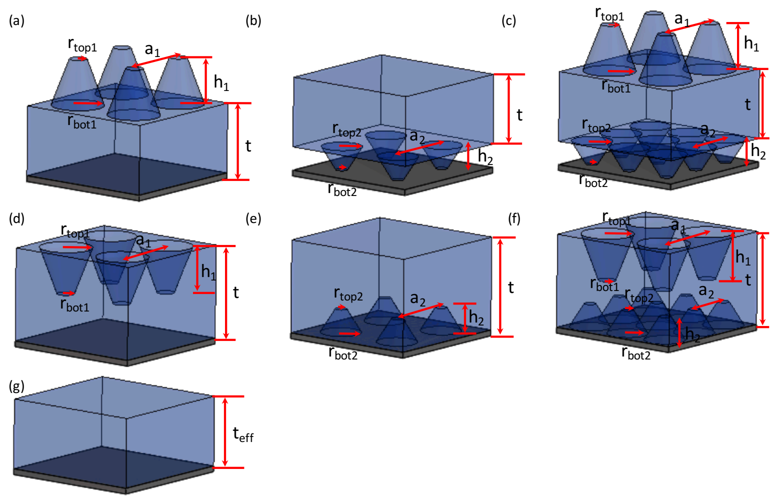

Figure 1: (a). Cone on the top (b). Cone on the bottom (c). Cone on both top and bottom (d). Cone hole on the top (e). Cone hole on the bottom (f). Cone hole on both top and bottom

1 Optimized Structures

Figure 1 shows all the structures that will be optimized.

1.1 Cone on the top

1.1.1 Four Variables Implementation

The bound constraint conditions are the same as before without the constraint for h_1. Let $\mathbf{x} = (r_{top1}, r_{bot1}, a_1, t)^T$.

1.1.2 Effective Thickness Constraint

a_{max} and t_{eff} are set by the user. To start with, we set $a_{max} = 4000$ nm, and $a_{min} = 100$ nm. If we set $a_{min} = 0$, we should recover previous results. The bound constraint conditions are the same as before without the constraint for h_1. Let $\mathbf{x} = (r_{top1}, r_{bot1}, a_1, t)^T$.

$$\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ 0 \end{pmatrix} \leq \mathbf{x} \leq \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ t_{eff} \end{pmatrix} \tag{1.1}$$

The linear inequality constraints are

$$2r_{top1} \leq a_1$$
$$2r_{bot1} \leq a_1$$

The linear inequality constraints are of the form $\mathbf{Ax} \leq \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & -1 & 0 \\ 0 & 2 & -1 & 0 \end{pmatrix} \mathbf{x} \leq \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{1.2}$$

The volume is unchanged during optimization, which results in the following derivation for the cone height h_1.

$$
\begin{aligned}
a_1^2 t_{eff} &= a_1^2 t + \frac{1}{3}\pi h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) \\
t &= t_{eff} - \frac{1}{3a_1^2}\pi h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) \\
h_1 &= \frac{3a_1^2 (t_{eff} - t)}{\pi (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1})} \qquad (1.3)
\end{aligned}
$$

$$
\boxed{h_1 = \frac{3a_1^2 (t_{eff} - t)}{\pi (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1})}} \qquad (1.4)
$$

The minimum h_1 occurs when $t = t_{eff}$. The maximum h_1 occurs when $t = 0$, $a_1 = a_{max}$, and $r_{top1} = r_{bot1} = a_{min}/2$. The input h_1 is constrained by the following condition and h_1 is always positive.

$$
0 \le h_1 \le \frac{4t_{eff}}{\pi} \frac{a_{max}^2}{a_{min}^2}.
$$

1.1.3 Total Thickness Constraint Implementation

Here we provide another method of setting constraints for optimization. Instead of constraining the optimization based on effective thickness, t_{eff}, we constrain the total thickness t_{tot} where $h_1 + t = t_{tot}$. Let $\mathbf{x} = (r_{top1}, r_{bot1}, a_1, t)^T$. a_{max} and t_{total} are set by the user. To start with, we set $a_{max} = 4000$ nm, $a_{min} = 100$ nm, $t_{total} = 1000 nm$. If we set $a_{min} = 0$, we should recover previous results. The bound constraints on the range of variables are

$$
\begin{aligned}
a_{min}/2 \le r_{top1} \le a_{max}/2 \\
a_{min}/2 \le r_{bot1} \le a_{max}/2 \\
a_{min} \le a_1 \le a_{max} \\
0 \le t \le t_{total}
\end{aligned}
$$

We can express the bound constrains in matrix form as

$$
\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ 0 \end{pmatrix} \le \mathbf{x} \le \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ t_{total} \end{pmatrix} \qquad (1.5)
$$

The linear inequality constraints are

$$
\begin{aligned}
2r_{top1} \le a_1 \\
2r_{bot1} \le a_1
\end{aligned}
$$

The linear inequality constraints are of the form $\mathbf{Ax} \le \mathbf{b}$.

$$
\begin{pmatrix} 2 & 0 & -1 & 0 \\ 0 & 2 & -1 & 0 \end{pmatrix} \mathbf{x} \le \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad (1.6)
$$

The summation of cone height h_1 and thin film thickness t should be equals to pre-setting t_{total}, which results in a different constraint from previous section.

$$\begin{aligned} h_1 + t &= t_{total} \\ h_1 &= t_{total} - t \end{aligned} \tag{1.7}$$

$$\boxed{h_1 = t_{total} - t} \tag{1.8}$$

From the equation above, we know the h_1 will be smaller than t_{total} by itself and it is always positive.

$$0 \leq h \leq t_{total} \tag{1.9}$$

No additional constraints must be implemented for h_1.

1.2 Cone on the bottom

1.2.1 Effective Thickness Constraint Implementation

The constraints are exactly the same as in the above case, except all the structures are on the bottom as opposed to the top. The bound constraint conditions are similar as before without the input variable h_2. Let $\mathbf{x} = (r_{top2}, r_{bot2}, a_2, t)^T$.

$$\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ 0 \end{pmatrix} \leq \mathbf{x} \leq \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ t_{eff} \end{pmatrix} \tag{1.10}$$

The linear inequality constraints are

$$\begin{aligned} 2r_{top2} &\leq a_2 \\ 2r_{bot2} &\leq a_2 \end{aligned}$$

The linear inequality constraints are of the form $\mathbf{Ax} \leq \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & -1 & 0 \\ 0 & 2 & -1 & 0 \end{pmatrix} \mathbf{x} \leq \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{1.11}$$

h_2 may be calculated from the other four variables.

$$h_2 = \frac{3a_2^2(t_{eff} - t)}{\pi(r_{top2}^2 + r_{bot2}^2 + r_{top2}r_{bot2})} \tag{1.12}$$

With the other constraints in place, the constraints on h_2 will automatically be satisfied. In this way, the optimization could be simplified.

1.2.2 Total Thickness Constraint Implementation

For this case, it is similar to the previous conetop structure, also there are four input variables, r_{top2}, r_{bot2}, a_2 and t. Let $\mathbf{x} = (r_{top2}, r_{bot2}, a_2, t)^T$. a_{max} and t_{total} are set by the user. To start with, we set $a_{max} = 4000$ nm, $a_{min} = 100$ nm, $t_{total} = 1000$ nm. If we set $a_{min} = 0$, we should recover previous results. The bound constraints on the range of variables are

$$\begin{aligned} a_{min}/2 \le r_{top2} \le a_{max}/2 \\ a_{min}/2 \le r_{bot2} \le a_{max}/2 \\ a_{min} \le a_2 \le a_{max} \\ 0 \le t \le t_{total} \end{aligned}$$

We can express the bound constrains in matrix form as

$$\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ 0 \end{pmatrix} \le \mathbf{x} \le \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ t_{total} \end{pmatrix} \tag{1.13}$$

The linear inequality constraints are

$$\begin{aligned} 2r_{top2} \le a_1 \\ 2r_{bot2} \le a_1 \end{aligned}$$

The linear inequality constraints are of the form $\mathbf{Ax} \le \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & -1 & 0 \\ 0 & 2 & -1 & 0 \end{pmatrix} \mathbf{x} \le \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{1.14}$$

The summation of cone height h_1 and thin film thickness t should be equals to pre-setting t_{total}, which results in a different constraint from previous section.

$$\begin{aligned} h_2 + t = t_{total} \\ h_2 = t_{total} - t \end{aligned} \tag{1.15}$$

From the equation above, we know the h_2 will be smaller than t_{total} by itself and it is always positive.

1.3 Cone on both top and bottom

Figure 1 (c) shows nanocone structures on both top and bottom of the thin film. For this complicated structure, we first have the case where we assume the pitches on the top and bottom are the same before relaxing this assumption.

1.3.1 Same Pitch on Both Top and Bottom

In this section, we make assumption that the periodicity of the cones on top a_1 and the periodicity of the cones on the bottom are equal to one another, or $a_1 = a_2 = a$.

I. **Seven Variables Implementation**

For this section, we are trying to reduce one more variable from the input variables, such as t. Thus the variables are r_{top1}, r_{top2}, r_{bot1}, r_{bot2}, a, h_1, and h_2.
Let $\mathbf{x} = (r_{top1}, r_{bot1}, r_{top2}, r_{bot2}, a, h_1, h_2)^T$.
a_{min}, a_{max} and t_{eff} are set by the user. To start with, we set $a_{max} = 4000$ nm,

a_{min} = 100 nm and t_{eff} = 1000nm. If we set $a_{min} = 0$, we should recover previous results. The bound constraints on the range of variables are

$$\begin{aligned}
a_{min}/2 \le r_{top1} \le a_{max}/2 \\
a_{min}/2 \le r_{bot1} \le a_{max}/2 \\
a_{min}/2 \le r_{top2} \le a_{max}/2 \\
a_{min}/2 \le r_{bot2} \le a_{max}/2 \\
a_{min} \le a \le a_{max} \\
0 \le h_1 \le \frac{4t_{eff}}{\pi} \\
0 \le h_2 \le \frac{4t_{eff}}{\pi}
\end{aligned}$$

We can express the bound constrains in matrix form as follow

$$\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ 0 \\ 0 \end{pmatrix} \le \mathbf{x} \le \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ \frac{4t_{eff}}{\pi} \\ \frac{4t_{eff}}{\pi} \end{pmatrix} \tag{1.16}$$

The linear inequality constraints are

$$\begin{aligned}
2r_{top1} \le a \\
2r_{bot1} \le a \\
2r_{top2} \le a \\
2r_{bot2} \le a
\end{aligned}$$

Linear inequality constraints are of the form $\mathbf{Ax} \le \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 2 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 2 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 2 & -1 & 0 & 0 \end{pmatrix} \mathbf{x} \le \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{1.17}$$

$$\begin{aligned}
a^2 t_{eff} &= a^2 t + \frac{1}{3}\pi h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) + \frac{1}{3}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \\
t &= t_{eff} - \frac{1}{3a^2}\pi h_1 (r_{top1}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) - \frac{1}{3a^2}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2})
\end{aligned} \tag{1.18}$$

$$\boxed{t = t_{eff} - \frac{1}{3a^2}\pi h_1 (r_{top1}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) - \frac{1}{3a^2}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2})} \tag{1.19}$$

The maximum t occurs when h_1 and h_2 are 0 or $t_{max} = t_{eff}$. [The minimum t occurs when...]

II. **Total Thickness Constraint Implementation**

For this section, we are trying to use another way to do with the constraints and reduce one more variable from the input variables, such as t. Thus the variables are r_{top1}, r_{top2}, r_{bot1}, r_{bot2}, a, h_1, and h_2.

Let $\mathbf{x} = (r_{top1}, r_{bot1}, r_{top2}, r_{bot2}, a, h_1, h_2)^T$.

a_{min}, a_{max} and t_{total} are set by the user. To start with, we set $a_{max} = 4000$ nm, $a_{min} = 100$ nm and $t_{total} = 1000$nm. If we set $a_{min} = 0$, we should recover previous results. The bound constraints on the range of variables are

$$\begin{aligned} a_{min}/2 &\leq r_{top1} \leq a_{max}/2 \\ a_{min}/2 &\leq r_{bot1} \leq a_{max}/2 \\ a_{min}/2 &\leq r_{top2} \leq a_{max}/2 \\ a_{min}/2 &\leq r_{bot2} \leq a_{max}/2 \\ a_{min} &\leq a \leq a_{max} \\ 0 &\leq h_1 \leq t_{total} \\ 0 &\leq h_2 \leq t_{total} \end{aligned}$$

We can express the bound constrains in matrix form as follow

$$\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ 0 \\ 0 \end{pmatrix} \leq \mathbf{x} \leq \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ t_{total} \\ t_{total} \end{pmatrix} \tag{1.20}$$

The linear inequality constraints are

$$\begin{aligned} 2r_{top1} &\leq a \\ 2r_{bot1} &\leq a \\ 2r_{top2} &\leq a \\ 2r_{bot2} &\leq a \\ h_1 + h_2 &\leq t_{total} \end{aligned}$$

Linear inequality constraints are of the form $\mathbf{Ax} \leq \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 2 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 2 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix} \mathbf{x} \leq \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ t_{total} \end{pmatrix} \tag{1.21}$$

All the structure is optimized in a range of thickness t_{total}, the input variables t and h_1 should be positve, thus h_2 is positive and automatically smaller than t_{total}.

$$\begin{aligned} h_1 + h_2 + t &= t_{total} \\ t &= t_{total} - h_1 - h_2 \end{aligned} \tag{1.22}$$

$$\boxed{t = t_{total} - h_1 - h_2} \tag{1.23}$$

Using linear constraint, we have

$$0 \leq t \leq t_{total} \tag{1.24}$$

[If we use 8 variables, can just implement everything with linear constraint. Think better to implement with $h_1 + h_2 + t = t_{total}$. Think if you implement the way you have written, t will be biased towards small values.]

1.3.2 Cone Arrays with Different Pitches on Both Top and Bottom

I. **Eleven Variables Implementation**

Figure 1 (c) shows nanocone structures on both top and bottom of a thin film. The variables are r_{top1}, r_{top2}, r_{bot1}, r_{bot2}, a_1, a_2, n_1, n_2 , h_1, h_2, and t.
Let $\mathbf{x} = (r_{top1}, r_{bot1}, r_{top2}, r_{bot2}, a_1, a_2, n_1, n_2, h_1, h_2, t)^T$.
a_{max}, n_{max} and t_{eff} are set by the user. n_1 and n_2 are integers. To start with, we set $a_{max} = 4000$ nm. We can set $a_{min} = 100$ nm. If we set $a_{min} = 0$, we should recover previous results. $n_{max} = \lfloor a_{max}/a_{min} \rfloor$, where $\lfloor\rfloor$ denotes the floor function. [Need to update this.]

The bound constraints on the range of variables are

$$\begin{aligned}
a_{min}/2 &\leq r_{top1} \leq a_{max}/2 \\
a_{min}/2 &\leq r_{bot1} \leq a_{max}/2 \\
a_{min}/2 &\leq r_{top2} \leq a_{max}/2 \\
a_{min}/2 &\leq r_{bot2} \leq a_{max}/2 \\
a_{min} &\leq a_1 \leq a_{max} \\
a_{min} &\leq a_2 \leq a_{max} \\
1 &\leq n_1 \leq \lfloor a_{max}/a_{min} \rfloor \\
1 &\leq n_2 \leq \lfloor a_{max}/a_{min} \rfloor \\
0 &\leq h_1 \leq \frac{4t_{eff}}{4+\pi} \\
0 &\leq h_2 \leq \frac{4t_{eff}}{4+\pi} \\
0 &\leq t \leq t_{eff}
\end{aligned}$$

We can express the bound constrains in matrix form as follow

$$\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ a_{min} \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \leq \mathbf{x} \leq \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ a_{max} \\ \lfloor a_{max}/a_{min} \rfloor \\ \lfloor a_{max}/a_{min} \rfloor \\ \frac{4t_{eff}}{4+\pi} \\ \frac{4t_{eff}}{4+\pi} \\ t_{eff} \end{pmatrix} \tag{1.25}$$

The linear inequality constraints are

$$\begin{aligned} 2r_{top1} &\leq a_1 \\ 2r_{bot1} &\leq a_1 \\ 2r_{top2} &\leq a_2 \\ 2r_{bot2} &\leq a_2 \end{aligned}$$

Linear inequality constraints are of the form $\mathbf{Ax} \leq \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \mathbf{x} \leq \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{1.26}$$

We can interpret a as $a = n_1 a_1 = n_2 a_2$, n_1 and n_2 must be positive integers and are the number of unit cells in a simulation cell. The volume must be unchanged during simulation:

$$\begin{aligned} a^2 t_{eff} &= a^2 t + \frac{1}{3}\pi n_1^2 h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) + \frac{1}{3}\pi n_2^2 h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \\ (n_1 a_1)^2 t_{eff} &= (n_1 a_1)^2 t + \frac{1}{3}\pi n_1^2 h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) + \frac{1}{3}\pi n_2^2 h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \\ t &= t_{eff} - \frac{1}{3a_1^2}\pi h_1 (r_{top1}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) - \frac{1}{3a_2^2}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \end{aligned}$$

The two nonlinear equality constraints are thus

$$n_1 a_1 = n_2 a_2 \tag{1.27}$$

$$t = t_{eff} - \frac{1}{3a_1^2}\pi h_1 (r_{top1}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) - \frac{1}{3a_2^2}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \tag{1.28}$$

The maximum t occurs when h_1 and h_2 are 0. $t = t_{eff}$
The maximum h_1 occurs when $h_2 = 0$, $t = h_{max}$ and $r_{top1} = r_{bot1} = a_1/2$.

$$h_1 \leq \frac{4t_{eff}}{4+\pi}$$

The maximum h_2 occurs when $h_1 = 0$, $t = h_{max}$ and $r_{top2} = r_{bot2} = a_2/2$.

$$h_2 \leq \frac{4t_{eff}}{4+\pi}$$

II. Ten Variables Implementation

In order to simplify the optimization, here we reduce one parameter from the input, such as, t. Then the remain variables are r_{top1}, r_{top2}, r_{bot1}, r_{bot2}, a_1, a_2, n_1, n_2 , h_1,and h_2.

Let $\mathbf{x} = (r_{top1}, r_{bot1}, r_{top2}, r_{bot2}, a_1, a_2, n_1, n_2, h_1, h_2)^T$. a_{max}, a_{min} and t_{eff} are set by the user. n_1 and n_2 are integers. To start with, we set $a_{max} = 4000$ nm,$a_{min} = 100$ nm and $t_{eff} = 1000$ nm. If we set $a_{min} = 0$, we should recover previous results. $n_{max} = \lfloor a_{max}/a_{min} \rfloor$, where $\lfloor\rfloor$ denotes the floor function.

The bound constraints on the range of variables are

$$\begin{aligned}
a_{min}/2 \leq r_{top1} &\leq a_{max}/2 \\
a_{min}/2 \leq r_{bot1} &\leq a_{max}/2 \\
a_{min}/2 \leq r_{top2} &\leq a_{max}/2 \\
a_{min}/2 \leq r_{bot2} &\leq a_{max}/2 \\
a_{min} \leq a_1 &\leq a_{max} \\
a_{min} \leq a_2 &\leq a_{max} \\
1 \leq n_1 &\leq \lfloor a_{max}/a_{min} \rfloor \\
1 \leq n_2 &\leq \lfloor a_{max}/a_{min} \rfloor \\
0 \leq h_1 &\leq \frac{4t_{eff}}{4+\pi} \\
0 \leq h_2 &\leq \frac{4t_{eff}}{4+\pi}
\end{aligned}$$

We can express the bound constrains in matrix form as follow

$$\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ a_{min} \\ 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \leq \mathbf{x} \leq \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ a_{max} \\ \lfloor a_{max}/a_{min} \rfloor \\ \lfloor a_{max}/a_{min} \rfloor \\ \frac{4t_{eff}}{4+\pi} \\ \frac{4t_{eff}}{4+\pi} \end{pmatrix} \tag{1.29}$$

The linear inequality constraints are

$$\begin{aligned} 2r_{top1} &\le a_1 \\ 2r_{bot1} &\le a_1 \\ 2r_{top2} &\le a_2 \\ 2r_{bot2} &\le a_2 \end{aligned}$$

Linear inequality constraints are of the form $\mathbf{Ax} \le \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \mathbf{x} \le \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{1.30}$$

We can interpret a as $a = n_1 a_1 = n_2 a_2$, n_1 and n_2 must be positive integers and are the number of unit cells in a simulation cell. The volume must be unchanged during simulation:

$$\begin{aligned} a^2 t_{eff} &= a^2 t + \frac{1}{3}\pi n_1^2 h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) + \frac{1}{3}\pi n_2^2 h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \\ (n_1 a_1)^2 t_{eff} &= (n_1 a_1)^2 t + \frac{1}{3}\pi n_1^2 h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) + \frac{1}{3}\pi n_2^2 h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \\ t &= t_{eff} - \frac{1}{3a_1^2}\pi h_1 (r_{top1}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) - \frac{1}{3a_2^2}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \end{aligned}$$

The two nonlinear equality constraints are thus

$$n_1 a_1 = n_2 a_2 \tag{1.31}$$

$$t = t_{eff} - \frac{1}{3a_1^2}\pi h_1 (r_{top1}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) - \frac{1}{3a_2^2}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \tag{1.32}$$

The maximum t occurs when h_1 and h_2 are 0. $t = t_{eff}$, in other case t is less than t_{total} automatically.

III. **Total Thickness Constraint Implementation**

1.3.3 Integer Optimization Implementation

`http://www.mathworks.com/help/gads/mixed-integer-optimization.html#bs1clc2`. n_1 and n_2 can be constrained to be integers by setting `IntCon = [8, 9]`. With integer constraints, there cannot be any linear equality constraints. One workaround is to include two linear inequality constraints. To include the nonlinear equality constraint, a small tolerance `tol` must be implemented, which allows the t to be within tol of the expression. `tol` is a small number.

$$n_1 a_1 - n_2 a_2 - tol \le 0 \tag{1.33}$$

$$-[n_1 a_1 - n_2 a_2] - tol \le 0 \tag{1.34}$$

$$t - t_{eff} - \frac{1}{3a_1^2}\pi h_1(r_{top1}^2 + r_{bot2}^2 + r_{top2}r_{bot2}) - \frac{1}{3a_2^2}\pi h_2(r_{top2}^2 + r_{bot2}^2 + r_{top2}r_{bot2}) - tol \le 0 \tag{1.35}$$

$$-\left[t - t_{eff} - \frac{1}{3a_1^2}\pi h_1(r_{top1}^2 + r_{bot2}^2 + r_{top2}r_{bot2}) - \frac{1}{3a_2^2}\pi h_2(r_{top2}^2 + r_{bot2}^2 + r_{top2}r_{bot2})\right] - tol \le 0 \tag{1.36}$$

1.3.4 Reduced Variable Integer Optimization Implementation

1.4 Cone hole on the top

1.4.1 Five Variables Implementation

Figure 1 (d) shows nanocone hole structures on the top of the thin film. The five input variables are r_{top1}, r_{bot1}, a_1, h_1, and t. Let $\mathbf{x} = (r_{top1}, r_{bot1}, a_1, h_1, t)^T$. a_{max} and t_{eff} are set by the user. To start with, we set $a_{max} = 4000$ nm. We can set $a_{min} = 100$ nm. If we set $a_{min} = 0$, we should recover previous results. The bound constraints on the range of variables are

$$\begin{aligned} a_{min}/2 \le r_{top1} &\le a_{max}/2 \\ a_{min}/2 \le r_{bot1} &\le a_{max}/2 \\ a_{min} \le a_1 &\le a_{max} \\ 0 \le h_1 &\le \frac{4t_{eff}}{4-\pi} \\ t_{eff} \le t &\le \frac{4t_{eff}}{4-\pi} \end{aligned}$$

We can express the bound constrains in matrix form as

$$\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ 0 \\ t_{eff} \end{pmatrix} \le \mathbf{x} \le \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ \frac{4t_{eff}}{4-\pi} \\ \frac{4t_{eff}}{4-\pi} \end{pmatrix} \tag{1.37}$$

The linear constraints are

$$\begin{aligned} 2r_{top1} &\le a_1 \\ 2r_{bot1} &\le a_1 \\ h_1 &\le t \end{aligned}$$

Linear inequality constraints are of the form $\mathbf{Ax} \le \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & -1 & 0 & 0 \\ 0 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 \end{pmatrix} x \le \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \tag{1.38}$$

The volume is unchanged during optimization, which results in a nonlinear constraint

$$
\begin{aligned}
a_1^2 t_{eff} &= a_1^2 t - \frac{1}{3}\pi h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) \\
h_1 &= \frac{3a_1^2(t - t_{eff})}{\pi(r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1})} \\
t &= t_{eff} + \frac{1}{3a_1^2}\pi h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1})
\end{aligned}
\tag{1.39}
$$

The maximum h_1 occurs when $t = h_{max}$, and $r_{top1} = r_{bot1} = a_1/2$

$$
\begin{aligned}
h_{max} &= \frac{3a^2(h_{max} - t_{eff})}{\pi(\frac{a^2}{4} + \frac{a^2}{4} + \frac{a^2}{4})} \\
h_{max} &= \frac{4t_{eff}}{4 - \pi}
\end{aligned}
$$

The maximum t occurs when $h_1 = t_{max}$, and $r_{top1} = r_{bot1} = a_1/2$

$$
t_{max} = \frac{4t_{eff}}{4 - \pi}
$$

1.4.2 Four Variables Implementation

For this section, we eliminate one inout variable. Say, h_1, Thus the remaining four input variables are r_{top1}, r_{bot1}, a_1, and t. Let $\mathbf{x} = (r_{top1}, r_{bot1}, a_1, t)^T$. a_{max} and t_{eff} are set by the user. To start with, we set $a_{max} = 4000$ nm.We can set $a_{min} = 100$ nm. If we set $a_{min} = 0$, we should recover previous results. The bound constraints on the range of variables are

$$
\begin{aligned}
a_{min}/2 \le r_{top1} &\le a_{max}/2 \\
a_{min}/2 \le r_{bot1} &\le a_{max}/2 \\
a_{min} \le a_1 &\le a_{max} \\
t_{eff} \le t &\le \frac{4t_{eff}}{4 - \pi}
\end{aligned}
$$

We can express the bound constrains in matrix form as

$$
\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ 0 \\ t_{eff} \end{pmatrix} \le \mathbf{x} \le \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ \frac{4t_{eff}}{4-\pi} \\ \frac{4t_{eff}}{4-\pi} \end{pmatrix}
\tag{1.40}
$$

The linear constraints are

$$
\begin{aligned}
2r_{top1} &\le a_1 \\
2r_{bot1} &\le a_1
\end{aligned}
$$

Linear inequality constraints are of the form $\mathbf{A}\mathbf{x} \leq \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & -1 & 0 \\ 0 & 2 & -1 & 0 \end{pmatrix} x \leq \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{1.41}$$

The volume is unchanged during optimization, which results in a nonlinear constraint

$$\begin{aligned} a_1^2 t_{eff} &= a_1^2 t - \frac{1}{3}\pi h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) \\ h_1 &= \frac{3a_1^2(t - t_{eff})}{\pi(r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1})} \\ t &= t_{eff} + \frac{1}{3a_1^2}\pi h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) \end{aligned} \tag{1.42}$$

The maximum t occurs when $h_1 = t_{max}$, and $r_{top1} = r_{bot1} = a_1/2$

$$t_{max} = \frac{4t_{eff}}{4 - \pi}$$

When $t = t_{eff}$, $h_1 = 0$. The lower bound on h_1 is recovered. At the same time, the maximum bound on h_1 could be satisfied by the linear constraint, $h_1 < t$ automatically. We give a brief proof here. We calculate h_1 from the above equation.

$$h_1 = \frac{3a_1^2(t - t_{eff})}{\pi(r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1})}$$

If we make the $\frac{3a_1^2(t-t_{eff})}{\pi(r_{top1}^2+r_{bot1}^2+r_{top1}r_{bot1})} \leq t$, we could get the upper bound for t, which is just the same constraint that we mentioned in this section. As a result, the constraint for $h_1 \leq t$ could be satisfied automatically.

1.4.3 Total Thickness Constraint Implementation

When the structure becomes cone hole on the top. Let $\mathbf{x} = (r_{top1}, r_{bot1}, a_1, h_1)^T$.$a_{max}$ and t_{total} are set by the user. To start with, we set $a_{max} = 4000$ nm, $a_{min} = 100$ nm and $t_{total} = 1000$ nm. The four input variables are r_{top1}, r_{bot1}, a_1, and h_1. The bound constraints on the range of variables are

$$\begin{aligned} a_{min}/2 \leq r_{top1} \leq a_{max}/2 \\ a_{min}/2 \leq r_{bot1} \leq a_{max}/2 \\ a_{min} \leq a_1 \leq a_{max} \\ 0 \leq h_1 \leq t_{total} \end{aligned}$$

We can express the bound constrains in matrix form as

$$\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ 0 \end{pmatrix} \leq \mathbf{x} \leq \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ t_{total} \end{pmatrix} \tag{1.43}$$

The linear constraints are

$$2r_{top1} \leq a_1$$
$$2r_{bot1} \leq a_1$$

Linear inequality constraints are of the form $\mathbf{Ax} \leq \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & -1 & 0 \\ 0 & 2 & -1 & 0 \end{pmatrix} x \leq \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \tag{1.44}$$

The thickness of the thin film is the fixed value by $t = t_{total}$. So $h_1 \leq t_{total}$ makes it satisfied $h_1 \leq t$

1.5 Cone hole on the bottom

1.5.1 Five Variables Implementation

Figure 1 (e) shows nanocone hole structures on the bottom of a thin film. The variables are r_{top2}, r_{bot2}, a_2, h_2 and t. Let $\mathbf{x} = (r_{top2}, r_{bot2}, a_2, h_2, t)^T$. a_{max} and t_{eff} are set by the user. To start with, we set $a_{max} = 4000$ nm. We can set $a_{min} = 100$ nm. If we set $a_{min} = 0$. The bound constraints on the range of variables are

$$a_{min}/2 \leq r_{top2} \leq a_{max}/2$$
$$a_{min}/2 \leq r_{bot2} \leq a_{max}/2$$
$$a_{min} \leq a_2 \leq a_{max}$$
$$0 \leq h_2 \leq \frac{4t_{eff}}{4-\pi}$$
$$t_{eff} \leq t \leq \frac{4t_{eff}}{4-\pi}$$

We can express the bound constrains in a matrix form as follows

$$\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ 0 \\ t_{eff} \end{pmatrix} \leq \mathbf{x} \leq \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ \frac{4t_{eff}}{4-\pi} \\ \frac{4t_{eff}}{4-\pi} \end{pmatrix} \tag{1.45}$$

The linear constraints are

$$2r_{top2} \leq a_2$$
$$2r_{bot2} \leq a_2$$
$$h_2 \leq t$$

Linear inequality constraints are of the form $\mathbf{Ax} \leq \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & -1 & 0 & 0 \\ 0 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 \end{pmatrix} x \leq \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \tag{1.46}$$

After optimization, the volume is unchanged. The nonlinear constraint is

$$a_2^2 t_{eff} = a_2^2 t - \frac{1}{3}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2})$$
$$h_2 = \frac{3a_2^2 (t - t_{eff})}{\pi (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2})} \tag{1.47}$$

The maximum h_2 occurs when $t = h_{max}$, and $r_{top2} = r_{bot2} = a_2/2$

$$h_{max} = \frac{4t_{eff}}{4 - \pi}$$

The maximum t occurs when $h_2 = t_{max}$, and $r_{top2} = r_{bot2} = a_2/2$

$$t_{max} = \frac{4t_{eff}}{4 - \pi}$$

1.5.2 Four Variables Implementation

Different from Cone on the Bottomstructure, in the Cone Hole Bottom structure, h_2 could be positive for sure. But we have to set the upper bound by $h_2 \leq t$. As a result, I think for this structure, five input variables method is necessary.

1.5.3 Total Thickness Constraint Implementation

When the structure becomes cone hole on the bottom. Let $\mathbf{x} = (r_{top2}, r_{bot2}, a_2, h_2, t)^T . a_{max}$ and t_{total} are set by the user. To start with, we set $a_{max} = 4000$ nm, $a_{min} = 100$ nm and $t_{total} = 1000$ nm. The five input variables are r_{top2}, r_{bot2}, a_2, h_2, and t. The bound constraints on the range of variables are

$$a_{min}/2 \leq r_{top2} \leq a_{max}/2$$
$$a_{min}/2 \leq r_{bot2} \leq a_{max}/2$$
$$a_{min} \leq a_2 \leq a_{max}$$
$$0 \leq h_2 \leq t_{total}$$

We can express the bound constrains in matrix form as

$$\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ 0 \end{pmatrix} \leq \mathbf{x} \leq \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ t_{total} \end{pmatrix} \tag{1.48}$$

The linear constraints are

$$2r_{top2} \leq a_2$$
$$2r_{bot2} \leq a_2$$

Linear inequality constraints are of the form $\mathbf{Ax} \leq \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & -1 & 0 \\ 0 & 2 & -1 & 0 \end{pmatrix} x \leq \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{1.49}$$

The thickness of the thin film is the fixed value by $t = t_{total}$.

1.6 Cone hole on both top and bottom

Figure 1(f) shows nanocone hole structures on both top and bottom of the thin film.For this complicated structure, we make two assumptions, symmetric and asymmetric cone on both sides.

1.6.1 Symmetric Cone on Both Top and Bottom

I. **Eight Variables Implementation**

In this section, we make assumption that the whole structure is symmetric, which mean equal amount cone structures on both sides. Let's consider the simple situation. To optimize the cone structures, we input the eight variables, r_{top1}, r_{top2}, r_{bot1}, r_{bot2}, a, h_1, h_2, and t. a_{min}, a_{max} and t_{eff} are set by the user. Let $\mathbf{x} = (r_{top1}, r_{bot1}, r_{top2}, r_{bot2}, a, h_1, h_2, t)^T$. To start with, we set $a_{max} = 4000$ nm, $a_{min} = 100$ nm. and $t_{eff} = 1000$ nm. If we set $a_{min} = 0$, we should recover previous results. The constraints on the range of variables are

$$
\begin{aligned}
a_{min}/2 \leq r_{top1} &\leq a_{max}/2 \\
a_{min}/2 \leq r_{bot1} &\leq a_{max}/2 \\
a_{min}/2 \leq r_{top2} &\leq a_{max}/2 \\
a_{min}/2 \leq r_{bot2} &\leq a_{max}/2 \\
a_{min} \leq a &\leq a_{max} \\
0 \leq h_1 &\leq \frac{4t_{eff}}{4-\pi} \\
0 \leq h_2 &\leq \frac{4t_{eff}}{4-\pi} \\
t_{eff} \leq t &\leq \frac{4t_{eff}}{4-\pi}
\end{aligned}
$$

We can express the bound constrains in matrix form as

$$
\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ 0 \\ 0 \\ t_{eff} \end{pmatrix} \leq \mathbf{x} \leq \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ \frac{4t_{eff}}{4-\pi} \\ \frac{4t_{eff}}{4-\pi} \\ \frac{4t_{eff}}{4-\pi} \end{pmatrix} \tag{1.50}
$$

The linear constraints are

$$
\begin{aligned}
2r_{top1} &\leq a \\
2r_{bot1} &\leq a \\
2r_{top2} &\leq a \\
2r_{bot2} &\leq a \\
h_1 &\leq t \\
h_2 &\leq t
\end{aligned}
$$

Linear inequality constraints are of the form $\mathbf{Ax} \leq \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \end{pmatrix} \mathbf{x} \leq \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{1.51}$$

After optimization, the volume is unchanged. The nonlinear constraints are thus,

$$\begin{aligned} a^2 t_{eff} &= a^2 t - \frac{1}{3}\pi h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) - \frac{1}{3}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \\ t &= t_{eff} + \frac{1}{3a^2}\pi h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) + \frac{1}{3a^2}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \end{aligned} \tag{1.52}$$

The maximum h_1 and h_2 occur when $h_2 = 0$, $t = h_{1max}$, $r_{top1} = r_{bot1} = a_1/2$

$$h_{1max} = \frac{4t_{eff}}{4 - \pi}$$

Similarly

$$h_{2max} = \frac{4t_{eff}}{4 - \pi}$$

The maximum t occurs when $h_1 + h_2 = t_{max}$, $r_{top1} = r_{bot1} = a_1/2$ and $r_{top2} = r_{bot2} = a_2/2$

$$t_{max} = \frac{4t_{eff}}{4 - \pi}$$

II. **Total Thickness Constraint Implementation**

In this section, we make assumption that the whole structure is symmetric, which mean equal amount cone structures on both sides. Let's consider another method of constraints. To optimize the cone structures, we input the eight variables, r_{top1}, r_{top2}, r_{bot1}, r_{bot2}, a, h_1, h_2, and t. a_{min}, a_{max} and t_{total} are set by the user. Let $\mathbf{x} = (r_{top1}, r_{bot1}, r_{top2}, r_{bot2}, a, h_1, h_2, t)^T$. To start with, we set $a_{max} = 4000$ nm, $a_{min} = 100$ nm. and $t_{total} = 1000$ nm. If we set $a_{min} = 0$, we should recover previous results. The constraints on the range of variables are

$$\begin{aligned} a_{min}/2 &\leq r_{top1} \leq a_{max}/2 \\ a_{min}/2 &\leq r_{bot1} \leq a_{max}/2 \\ a_{min}/2 &\leq r_{top2} \leq a_{max}/2 \\ a_{min}/2 &\leq r_{bot2} \leq a_{max}/2 \\ a_{min} &\leq a \leq a_{max} \\ 0 &\leq h_1 \leq t_{total} \\ 0 &\leq h_2 \leq t_{total} \end{aligned}$$

We can express the bound constrains in matrix form as

$$\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ 0 \\ 0 \end{pmatrix} \leq \mathbf{x} \leq \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ t_{total} \\ t_{total} \end{pmatrix} \tag{1.53}$$

The linear constraints are

$$\begin{aligned} 2r_{top1} &\leq a \\ 2r_{bot1} &\leq a \\ 2r_{top2} &\leq a \\ 2r_{bot2} &\leq a \\ h_1 &\leq t_{total} \\ h_2 &\leq t_{total} \end{aligned}$$

Linear inequality constraints are of the form $\mathbf{Ax} \leq \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 2 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \mathbf{x} \leq \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ t_{total} \\ t_{total} \end{pmatrix} \tag{1.54}$$

During the optimization, the thickness of thin film is unchanged.

$$t = t_{total} \tag{1.55}$$

1.6.2 Asymmetric Cone on Both Top and Bottom

I. **Eleven Variables Implementation**
In this section, we make assumption that the whole structure is not symmetric, which means no equality amount cone structures on both sides. To optimize the cone structures, the input variables are, r_{top1}, r_{top2}, r_{bot1}, r_{bot2}, a_1, a_2, n_1, n_2, h_1, h_2, and t. a_{min}, a_{max} and t_{eff} are set by the user. Let $\mathbf{x} = (r_{top1}, r_{bot1}, r_{top2}, r_{bot2}, a_1, a_2, n_1, n_2, h_1, h_2, t)^T$. To start with, we set $a_{max} = 4000$ nm, $a_{min} = 100$ nm. and $t_{eff} = 1000$ nm. If we set $a_{min} = 0$, we should recover previous results.

The constraints on the range of variables are

$$
\begin{aligned}
a_{min}/2 &\leq r_{top1} \leq a_{max}/2 \\
a_{min}/2 &\leq r_{bot1} \leq a_{max}/2 \\
a_{min}/2 &\leq r_{top2} \leq a_{max}/2 \\
a_{min}/2 &\leq r_{bot2} \leq a_{max}/2 \\
a_{min} &\leq a_1 \leq a_{max} \\
a_{min} &\leq a_2 \leq a_{max} \\
1 &\leq n_1 \leq \lfloor a_{max}/a_{min} \rfloor \\
1 &\leq n_2 \leq \lfloor a_{max}/a_{min} \rfloor \\
0 &\leq h_1 \leq \frac{4t_{eff}}{4-\pi} \\
0 &\leq h_2 \leq \frac{4t_{eff}}{4-\pi} \\
t_{eff} &\leq t \leq \frac{4t_{eff}}{4-\pi}
\end{aligned}
$$

We can express the bound constrains in matrix form as

$$
\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ a_{min} \\ 1 \\ 1 \\ 0 \\ 0 \\ t_{eff} \end{pmatrix} \leq \mathbf{x} \leq \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ a_{max} \\ \lfloor a_{max}/a_{min} \rfloor \\ \lfloor a_{max}/a_{min} \rfloor \\ \frac{4t_{eff}}{4-\pi} \\ \frac{4t_{eff}}{4-\pi} \\ \frac{4t_{eff}}{4-\pi} \end{pmatrix} \tag{1.56}
$$

The linear constraints are

$$
\begin{aligned}
2r_{top1} &\leq a_1 \\
2r_{bot1} &\leq a_1 \\
2r_{top2} &\leq a_2 \\
2r_{bot2} &\leq a_2 \\
h_1 &\leq t \\
h_2 &\leq t
\end{aligned}
$$

Linear inequality constraints are of the form $\mathbf{Ax} \leq \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \end{pmatrix} \mathbf{x} \leq \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{1.57}$$

We can interpret a as $a = n_1 a_1 = n_2 a_2$, n_1 and n_2 must be positive integers and are the number of unit cells in a simulation cell.

After optimization, the volume is unchanged.

$$\begin{aligned} a^2 t_{eff} &= a^2 t - \frac{1}{3}\pi n_1^2 h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) - \frac{1}{3}\pi n_2^2 h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \\ a_1^2 t_{eff} &= a_1^2 t - \frac{1}{3}\pi h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) - \frac{a_1^2}{3a_2^2}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \\ h_1 &= \frac{3a_1^2 (t - t_{eff})}{\pi (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1})} - \frac{a_1^2 h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2})}{a_2^2 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1})} \\ h_2 &= \frac{3a_2^2 (t - t_{eff})}{\pi (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2})} - \frac{a_2^2 h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1})}{a_1^2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2})} \\ t &= t_{eff} + \frac{1}{3a_1^2}\pi h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) + \frac{1}{3a_2^2}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \end{aligned}$$

The nonlinear constraints are thus,

$$n_1 a_1 = n_2 a_2 \tag{1.58}$$

$$t = t_{eff} + \frac{1}{3a_1^2}\pi h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) + \frac{1}{3a_2^2}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) \tag{1.59}$$

The maximum h_1 and h_2 occur when $h_2 = 0$, $t = h_{1max}$, $r_{top1} = r_{bot1} = a_1/2$

$$h_{1max} = \frac{4t_{eff}}{4 - \pi}$$

Similarly

$$h_{2max} = \frac{4t_{eff}}{4 - \pi}$$

The maximum t occurs when $h_1 + h_2 = t_{max}$, $r_{top1} = r_{bot1} = a_1/2$ and $r_{top2} = r_{bot2} = a_2/2$

$$t_{max} = \frac{4t_{eff}}{4 - \pi}$$

II. **Total Thickness Constraint Implementation** In this section, we make assumption that the whole structure is not symmetric, which means no equal amount cone structures on both sides. Apply another method of constraint. To optimize the cone structures, the input variables are, r_{top1}, r_{top2}, r_{bot1}, r_{bot2}, a_1, a_2, n_1, n_2, h_1, h_2, and t. a_{min}, a_{max} and t_{total} are set by the user. Let $\mathbf{x} = (r_{top1}, r_{bot1}, r_{top2}, r_{bot2}, a_1, a_2, n_1, n_2, h_1, h_2, t)^T$. To start with, we set $a_{max} = 4000$ nm, $a_{min} = 100$ nm. and $t_{total} = 1000$ nm. If we set $a_{min} = 0$, we should recover previous results.

The constraints on the range of variables are

$$
\begin{aligned}
a_{min}/2 \leq r_{top1} &\leq a_{max}/2 \\
a_{min}/2 \leq r_{bot1} &\leq a_{max}/2 \\
a_{min}/2 \leq r_{top2} &\leq a_{max}/2 \\
a_{min}/2 \leq r_{bot2} &\leq a_{max}/2 \\
a_{min} \leq a_1 &\leq a_{max} \\
a_{min} \leq a_2 &\leq a_{max} \\
1 \leq n_1 &\leq \lfloor a_{max}/a_{min} \rfloor \\
1 \leq n_2 &\leq \lfloor a_{max}/a_{min} \rfloor \\
0 \leq h_1 &\leq t_{total} \\
0 \leq h_2 &\leq t_{total}
\end{aligned}
$$

We can express the bound constrains in matrix form as

$$
\begin{pmatrix} a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min}/2 \\ a_{min} \\ a_{min} \\ 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \leq \mathbf{x} \leq \begin{pmatrix} a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max}/2 \\ a_{max} \\ a_{max} \\ \lfloor a_{max}/a_{min} \rfloor \\ \lfloor a_{max}/a_{min} \rfloor \\ t_{total} \\ t_{total} \end{pmatrix} \tag{1.60}
$$

The linear constraints are

$$
\begin{aligned}
2r_{top1} &\leq a_1 \\
2r_{bot1} &\leq a_1 \\
2r_{top2} &\leq a_2 \\
2r_{bot2} &\leq a_2 \\
h_1 &\leq t_{total} \\
h_2 &\leq t_{total}
\end{aligned}
$$

Linear inequality constraints are of the form $\mathbf{Ax} \leq \mathbf{b}$.

$$\begin{pmatrix} 2 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \mathbf{x} \leq \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ t_{total} \\ t_{total} \end{pmatrix} \tag{1.61}$$

We can interpret a as $a = n_1 a_1 = n_2 a_2$, n_1 and n_2 must be positive integers and are the number of unit cells in a simulation cell.

After optimization, the volume is unchanged. During the optimization, the thickness of thin film is unchanged.

$$t = t_{total} \tag{1.62}$$

1.6.3 Matlab Implementation

n_1 and n_2 can be constrained to be integers using `IntCon = [7, 8]` where 7 and 8 are the indices for n_1 and n_2 into the $\mathbf{x}$ vector.

For nonlinear equality constraint, it is represented by two inequality constraints with a small tolerance *tol*.

$$n_1 a_1 - n_2 a_2 - tol \leq 0 \tag{1.63}$$

$$-[n_1 a_1 - n_2 a_2] - tol \leq 0 \tag{1.64}$$

$$a_1^2 t_{eff} - a_1^2 t + \frac{1}{3}\pi h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) + \frac{a_1^2}{3a_2^2}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2}) - tol \leq 0 \tag{1.65}$$

$$-\left[a_1^2 t_{eff} - a_1^2 t + \frac{1}{3}\pi h_1 (r_{top1}^2 + r_{bot1}^2 + r_{top1} r_{bot1}) - \frac{a_1^2}{3a_2^2}\pi h_2 (r_{top2}^2 + r_{bot2}^2 + r_{top2} r_{bot2})\right] - tol \leq 0 \tag{1.66}$$

2 General Matlab Implementation

2.1 Writing Lumerical Objects

When an object is created in Lumerical, the default values are always the same. Thus, when the object is created in Matlab, we only set values that are different from the default.

2.2 Objects

I. Constants

   A. `@UnitConversions`, e.g. `NMtoM = 1e-9`, `HztoTHZ = 1e-12`

   B. `@LightConstants`

II. Objects

A. `@Model`
   i. `Structures`
   ii. `Source`
   iii. `Monitor1`
   iv. `Monitor2`
   v. `SimulationCell`

B. `@Source`
   i. `@PlaneSource`
      a) `@GeneralTab`
      b) `@GeneralTabType`
      c) `@GeometryTab`
         `X = 0`
         `XSpan = 1.8e-5`
         `XMin`
         `XMax`
         `Y = 0`
         `YSpan = 1.8e-5`
         `YMin`
         `YMax`
         `Z = 0`
         `ZSpan`
         `ZMin`
         `ZMax`
      d) `@BeamOptionTab`
      e) `@FrequencyWavelength`

```
classdef Source < matlab.System
  properties (Logical)
    OverrideGlobalSourceSettings
  end
```

`WavelengthMin`
`WavelengthMax`
`WavelengthCenter`
`WavelengthSpan`
`FrequencyMin`
`FrequencyMax`
`FrequencyCenter`
`FrequencySpan`
`Frequency`
`Pulselength`
`Offset`
`Bandwith`

C. `@DFTMonitor`

i. `@GeneralTab`

ii. `@GeneralTabType`

iii. `@GeometryMonitorTab`
```
MonitorType: 2D Z-normal
X = 0
XMax
XMin
XSpan = 1.8e-5
Y = 0
YMax
YMin
YSpan = 1.8e-5
Z
ZMax
ZMin
ZSpan
DownSampleX = 1
DownSampleY = 1
DownSampleZ
```

iv. `@DataToRecordTab`
```
StandardFourierTransform
PartialSpectralAverage
TotalSpectralAverage
OutputEx = 1
OutputEy = 1
OutputEz = 1
OutputHx = 1
OutputHy = 1
OutputHz = 1
OutputPx = 1
OutputPy = 1
OutputPz = 1
OutputPower = 1
```

v. `@AdvancedMonitorTab`
```
SpatialInterpolation
Overide
```

D. `@FDTDSimulation`

i. `@GeneralTab`

ii. `@GeneralTabType`

iii. `@MeshSetting`

a) `@AutoNonUniform` `MeshAccuracy` // `MinMeshStep`
```
MeshRefinement
DtStabilityFactor
Meshingrefinement
```

iv. `@BoundaryCondition` `XMinBc`
`XMaxBc`
`YMinBc`
`YMaxBc`
`ZMinBc`
`ZMaxBc`

v. `@GeometryFDTDTab` `X`
`XSpan`
`XMin`
`XMax`
`Y`
`YSpan`
`YMin`
`YMax`
`Z`
`ZSpan`
`ZMin`
`ZMax`

E. **Cone on the top**

The variables are `rTop1, rBot1, a1, h1,` and `t.`

Introduce variable `RegionSpan` (TBD = value to be determined) to represent the Region Span and we also set the bottom of the structure as the xOy plane. Then we could set the source geometry by three variables: `xMin`, `xMax`, `zConeTop`

ReSpan = TBD
XMin = -ReSpan/2
XMax = ReSpan/2
$Z_{ConeTop} = L_1/2 + h_1 {+} t$

F. `@DFTMonitor`. Two monitors, one is for reflection, the other one is for transmission we also set the bottom of the structure as the xOy plane. zSpan is the region extended in z-axis

OverriderGlobalMonitorSetting = 1
FrequencyPoints = Maybe 1000

i. `@GeneralTab`
   a) `SimulationType`
   b) `MinWavelength`
   c)

ii. `@GeometryTab`

iii. Reflection Monitor ReMonitorX = ReSpan
ReMonitorY = ReSpan
ReMonitorZ = $L{+}h_1{+}t$

iv. Transmission Monitor ReMonitorX = ReSpan
ReMonitorY = ReSpan
ReMonitorZ = -($zSpan$ - $2M$ - L_1 -h_1 - t)

2.3 Constraint conditions implementation

There are six optimized structures. Two of them include the integer programming. The other four structures do not.

2.3.1 Optimization with integer constraints

For those applying the integer programming, we introduce `IntCon` in the optimization. `x = ga(fitnessfcn, nVars, A, b, [], [], LB, UB, nonlcon, IntCon, option)`. Note here, for the Genetic Algorithm output, when there are integer constraints, ga does not accept linear or non-linear equality constraints, only inequality constraints.

I. Input Argument. `fitnessfcn`: the fitness function
   `nVars`: Positive integer representing the number of variables in the problem.
   `A` is the matrix and b is a vector.
   `Aeq`: Matrix for linear equality constraints of the form Aeq*x = beq.
   LB and UB: Vector of lower and upper bounds.
   IntCon: Vector of positive integers. When IntCon is not empty. Aeq and beq must be empty, which means no linear equality allowed in this situation. There are also some predetermined settings:
   effectiveThickness or t_{eff} = 1000 nm
   amax = 2000 nm

II. Output Argument. x: Best point that ga located during its iterations.
   fval: fitness function evaluated at x
   exitflag: giving the signal to stop the iterating.

III. Structure I, II
   Not applying IntCon and nonlinear constraint, we could set `[x,fval,exitFlag]=ga(@(x)objFnc(x, effectiveThickness),nVariables,A,b,[],[], lowerBound,upperbound,[], gaoptions);` If there is no bound constraints, set `LB = [], UB = [].` and `nVariables = size(A,1)` or we just set it the number of variables. We also need to create the first generation by createFcn and load the first generation that we specify.

IV. Structure IV, V
   Similarly, not applying IntCon and nonlinear constraint, we could set
   `[x,fval,exitFlag]=ga(@(x)objFnc(x, effectiveThickness),4,A,b,[],[],lowerBound ,upperbound,[], gaoptions);`
   If there is no bound constraints, set `LB = [], UB = [].` In this case, we need to set the lower bound due to the geometry requirement: `lb = [0; 0; 0; effecttiveThickness ]`

2.3.2 Naming Convention

For the filenames, we could make it base on the input settings.
rTop(value)+rBot(value)+a1(value)+a2(value)+t(value)