We have an infinite slab with height $z = h$ and index n_0 cladded with index $n_1 < n_0$. A wave with frequency $f = c/\lambda$ propagates in the x direction and encounters a perturbation—a notch cut into the infinite slab defined in the x-z plane and constant for all y (approximately). This notch is defined by a width w, a depth e, and sidewall angle θ. The behavior of the wave and the notch is a function of all variables, but in general h, n_0, n_1, λ, e, and θ are dependent upon our goal, material, and process, and thus can be considered 'fixed' variables that we have no control over. We do, however, have control over w, along with the position of the notch x, and we will use this to optimize the properties of our sequence of notches: our grating coupler.

The behavior of a single notch is defined by four quantities, as a function of w:

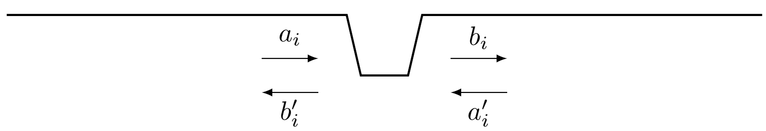
- the transmission of the notch $T = t^2$,
- the reflection of the notch $R = r^2$,
- the downward scatter from the notch $S_d = s_d^2$, and
- the upward scatter from the notch $S_u = s_u^2$.

The uppercase and lowercase variables represent power and amplitude, respectively. We measure power in experiment and simulation, but to fully understand the interference properties of a grating, we must consider the amplitude of our wave. If we have a wave propagating in the forward direction with amplitude a_i incident on a notch with width w_i,

- the forward propagating amplitude will be $b_i = ta_i$,
- the backward propagating amplitude will be $b'_i = ra_i$,
- the amplitude scattered upward will be $c_i = s_u a_i$, and
- the amplitude scattered downward will be $d_i = s_d a_i$.

Now let's consider that we also have a backward propagating wave a'_i incident on the notch. In this case,

- the forward propagating amplitude will be $b_i = ta_i + r^* a'_i$,
- the backward propagating amplitude will be $b'_i = ra_i + t^* a'_i$,
- the amplitude scattered upward will be $c_i = s_u(a_i + a'_i)$, and
- the amplitude scattered downward will be $d_i = s_d(a_i + a'_i)$.



Notice that this can be represented by a matrix:

$$\begin{bmatrix} a_i \\ b'_i \end{bmatrix} = \begin{bmatrix} 1/t & r^*/t \\ r/t & \frac{|t|^2+|r|^2}{t} \end{bmatrix} \begin{bmatrix} b_i \\ a'_i \end{bmatrix} = S(w_i) \begin{bmatrix} b_i \\ a'_i \end{bmatrix}$$

where b_i and a'_i are the forward- and backward- propagating amplitudes to the right of the notch and a_i and b'_i are that of the left of the notch[1]. As a rule of thumb in this notation, as are incident and bs are outgoing while primes are backward propagating and nonprimes are forward propagating.

Now let us consider multiple notches. Suppose that the ith and $(i+1)$th notches are separated by a distance L_i. Then, the amplitudes will obey the equation

$$\begin{aligned} a_{i+1} &= \varphi(L_i) b_i, \\ a'_i &= \varphi(L_i) b'_{i+1} \end{aligned}$$

where $\varphi(L_i) = \exp(2\pi i n_{eff} L_i/\lambda)$ is the phase evolution in the slab for the distance L_i and n_{eff} is effective index of the slab (we assume propagation loss is negligible and n_{eff} is real). That is,

$$\begin{bmatrix} b_i \\ a'_i \end{bmatrix} = \begin{bmatrix} \varphi^*(L_i) & 0 \\ 0 & \varphi(L_i) \end{bmatrix} \begin{bmatrix} a_{i+1} \\ b'_{i+1} \end{bmatrix} = \phi(L_i) \begin{bmatrix} a_{i+1} \\ b'_{i+1} \end{bmatrix}$$

[1] The proof is left as an exercise for the reader... :)

We want to see how this system behaves as a whole. Suppose the only light entering the system is incident and forward propagating on the 1st notch with amplitude a_1. No other light enters the system–specifically backward propagating through the last, Nth notch. That is $a'_N = 0$. If we normalize to the amplitude transmitted though the entire grating, i.e. $b_N = 1$, then we can backward-propogate to find all of the amplitudes everywhere. For instance, the amplitudes at the mth notch with $m < N$ are:

$$\begin{bmatrix} b_m \\ a'_m \end{bmatrix} = \phi(L_m) \left[\prod_{i=m+1}^{N-1} S(w_i)\phi(L_i) \right] S(w_N) \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

$$\begin{bmatrix} a_m \\ b'_m \end{bmatrix} = \left[\prod_{i=m}^{N-1} S(w_i)\phi(L_i) \right] S(w_N) \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

We also can determine the upward scattering amplitudes (normalized to the input a_1) at each notch

$$s_m = s_u(w_m)(a_m + a'_m)/a_1.$$

Lastly, note that each notch m is centered at

$$x_m = \left[\sum_{i=1}^{m-1} L_i + w_i \right] + w_m/2$$

and has a 'domain' of length

$$d_m = w_m + (L_{m-1} + L_m)/2$$

where $L_0 = L_1$ and $L_N = L_{N-1}$ and $x_0 = -d_1/2$.

Now, we want to evaluate the performance of the grating. For best results, the scattered amplitude will be in the shape of a gaussian

$$E(x) = \exp\left(-x^2/W^2\right)$$

where

$$W = \frac{\lambda}{\pi\,\mathrm{NA}}$$

is the waist of gaussian beam with wavelength λ and numerical aperture $\mathrm{NA} = n_0 \sin\Theta$ where Θ is the divergence angle of the beam. For early simulations, we will match to an objective with NA = .2. We can approximate the overlap between our arrayed scatterers and the ideal gaussian via

$$\gamma = \left| \sum_{i=1}^{N} \frac{s_i}{d_i} E(x_i - X) d_i \right|^2$$

where X is the 'center' of the scattered power which maximizes γ. We want to maximize γ while minimizing the reflected power $|b'_1/a_1|^2$, the transmitted power $|1/a_1|^2$, and downward scatter (computed similarly to upward). We do this by optimizing L_i and w_i via simulated annealing.