Re: Iterative Self-Consistent Fourier Functional Coating Synthesis.

Introduction.

Concepts and algorithms are discussed for direct synthesis of inhomogeneous layer structures directly from required target reflection amplitudes.

For a system of artificial, totally non-interacting interfaces, the relation between the reflectance amplitude and refractive index profile is,

$$\frac{1}{2n_{NI}}\frac{dn_{NI}}{dz} = \int r_{NI}(k)e^{ikz}dk = F_{NI}[r_{NI}]. \tag{1}$$

By non-interacting, it is meant that there are no internal reflections between boundaries in the layers, and optical thickness is introduced only as the phase factor in the integrand, relative to the front surface of the structure. Equation 1 is exact under those conditions. The *z* is twice the optical thickness, $k = 2\pi/\lambda$, F_{NI} [*r*] is the non-interacting functional of *r*.

If targets for the reflection amplitude of an interacting (real) system are inserted into Equation 1

$$\frac{1}{2\tilde{n}}\frac{d\tilde{n}}{dz} = \int r_I(k)e^{ikz}dk = F_{NI}[r_I], \tag{2}$$

the indices returned will ne non-physical and must be scaled. One option for the scaling is

$$\tilde{n} \to n_{\min} + (\tilde{n} - \tilde{n}_{\min})\frac{n_{\max} - n_{\min}}{\tilde{n}_{\max} - \tilde{n}_{\min}} \tag{3}$$

where $n_{\min,\,\max}$ are the max and minimum scaled indices permitted in the final design.

When the $\tilde{n}$ are evaluated with matrices, an error *Z* always results,

$$r_M\{\tilde{n}\} = r_I + Z, \tag{4}$$

where r_M is the reflection amplitude from a matrix evaluation of $\tilde{n}$.

Functional Concept.

The many-interacting interface problem will now be "mapped" onto one of a non-interacting interface problem.

It will now be shown that a functional exists that reproduces the index profile n_M which when evaluated with matrices, results in the target interacting reflectance amplitude, which has the form,

$$\frac{1}{2n_M}\frac{dn_M}{dz} = \int (r_I(k) - Z^0[r_I])e^{ikz}dk = F_{NI}[r_I] + E_I[r_I]. \tag{5}$$

The use of the notation Z^0 will become apparent momentarily. In Equation 4, the non-interacting and interacting aspects of the problem have been separated. If the functional E_I were known, it would be formally exact.

The proof is as follows:

Consider an iterative process of evaluating the following equation,

$$\frac{1}{2n^{i+1}}\frac{dn^{i+1}}{dz} = \int r_M^i\{n^i\}e^{ikz}dk. \tag{6}$$

The $r_M^i\{n^i\}$ is the reflectance amplitude of a matrix evaluation of the index profile produced in iteration *i* of the process. The relation between the iterations reflectance amplitudes defines the error,

$$r_M^{i+1}\{n^{i+1}\} - Z^{i+1}[r_M^i\{n_i\}] = r_M^i\{n^i\} \tag{7}$$

If one had wanted to produce $r_M^{i+1}\{n^{i+1}\}$ then substitution of Equation 7 into Equation 6 would have produced the required index profile for it.

So, if we start the process on iteration *i=0* with targets r_I and we know exactly the error to subtract Z^0 then evaluation of Equation 5 will produce an index profile, which when evaluated with matrices, produces the target reflectance amplitude r_I.

In order to know the $Z^{i+1}[r_M^i\{n_i\}]$ to subtract off, one must know exactly the functional and the index profile you are trying to produce at the onset – you must know the answer before you begin.

The separation of interacting and non-interacting behavior, introduction of approximate functionals, and self-consistent field solutions (in which the fields influencing your system depend on the particle density you are trying to solve for in the first place) are familiar problems in many-body theory (Hartree-Fock, Kohn-Sham).

Calling the term in parenthesis of Equation 5 (out of tradition), *Q(k)* = $r_I(k) - Z^0[r_I]$, and integrating both sides with respect over *z=0* to *z=z'* and dropping the prime after integration gives

$$n(z) = \exp\left[\int \frac{r_I(k) - Z^0[r_I]}{k} \sin(-kz) dk\right]. \quad (8)$$

Numerical results are achieved in effect by taking the integral back to a sum with a sufficiently small Δk,

$$n(z) = \exp\left[\sum_k \frac{r_I(k) - Z^0[r_I]}{k} \sin(-kz)\Delta k\right] \quad (9)$$

Finally, since phase information is typically not provided as a target,

$$n(z) = \exp\left[\sum_k \frac{R_I^{1/2}(k) - Z^0[R_I^{1/2}]}{k} \sin(-kz)\Delta k\right] \quad (10)$$

Equation 10 constitutes a seemingly confounded approximation. Recall that in the derivation of Equation 1 that index profile logarithmic derivative is the inverse transform of

$$r_{NI}(k) = \sum_z \frac{1}{2n_{NI}} \frac{dn_{NI}}{dz} e^{-ikz} \Delta z \Rightarrow \int \frac{1}{2n_{NI}} \frac{dn_{NI}}{dz} e^{-ikz} dz\,. \quad (11)$$

Thus $r_{NI}(k)$ still contains phase information and is a complex number. However, all of the same arguments could have been made with $r_M\{n\}$ and r_I replaced by $R_M\{n\}^{1/2}$ and $R_I^{1/2}$. The reason is that phase information is reinserted through the error Z and the matrix evaluations of n that comprise it. The functional itself is non-unique. The use of r or $R^{1/2}$ in all the arguments dictates the form of the functional, and in using R, we are simply selecting one of the non-unique functional choices that is convenient for us, because we do not have phase information. The transition from $r \Rightarrow R^{1/2}$ turns out to be a reasonable one, based on *a posteriori* evidence.

Noting equation 8,

$$n(z) = \exp\left[\int \frac{r_I(k) - Z^0[r_I]}{k} \sin(-kz) dk\right] = n_{NI(I)} n_Z \quad (12)$$

The notation $n_{I(NI)}$ denotes the index derived from targets for an interacting layer structure using the transform for non-interacting interfaces, and n_Z is the index adjustment formed from the difference between interacting (with matrices) and the non-interacting treatment.

Iterations to self-consistency will now be discussed.

Proposed Solution by Self-Consistent Iteration.

This is the most practical and direct approach.

It is postulated that the system can be solved by a method of iterating to self-consistency, without knowledge of the functional at all.

There are a number of ways this might be done. One way is as follows:

1. The targets $r_I(k)$ are evaluated in Equation 2 and the error is extracted in Equation 4. This error is actually Z^1.
2. The first approximation $Z^0 = Z^1$ is made.
3. Equation 5 is then evaluated with the argument $r_I - Z^0$, yielding an index profile n.
4. $r_M\{n\}$ is evaluated, which is supposed (hoped) to be closer to r_I.
5. The new error is $Z^1 = r_M\{n\} - (r_I - Z^0)$.
6. Return to step 2, or stop when the difference between $|Z_0 - Z_1|$ falls below a threshold, that is, when $r_M\{n\} = r_I$ the error stops evolving.

In this procedure, the error on iteration u adds to

$$Z^u = \sum_i (r_M^i - r_I), \tag{12}$$

and so is cumulative.

There may be better ways of finding Z_0. Basically, what the routine does is a single "forward" iteration in finding the first Z^1, such that we need not guess a starting point.

Proposed Solution by Extrapolation with Orthoganol Functions.

1. Use as targets $r^0=r_I$ in Equation 6, substituting back in the new r_M each time and iterating. The iterations will be approaching the wrong answer.
2. Collect the error function $Z^{i>0}$ on each iteration for analysis.
3. After running N iterations, stop.
4. Expand each $Z^{i>0}$ in a basis of orthoganol functions, Equation 13.
5. Fit the coefficients for iterations $i>0$ to polynomials as functions of i.
6. Extrapolate the coefficients to $i=0$.
7. Construct Z^0 using Equation 13.
8. Go to the self-consistency algorithm *OR*
9. Go back to step 1 but use $r^0=r_I - Z^0$ as the initial input.

$$Z^i = \sum_n \langle n | Z^i \rangle | n \rangle = \sum_n c_n^i \phi_n \tag{13}$$

Proposed Solution by Approximate Functional Construction.

This idea is far more nebulous. It would have to be done off-line, the functional developed, then attempted to be used generally, for many other problems.

1. Use as targets $r^0=r_I$ in Equation 6, substituting back the new r_M each time and iterating. The iterations will be approaching the wrong answer.
2. Collect the error function $Z^{i>0}$ on each iteration for analysis.
3. After running *N* iterations, stop.
4. One now has a family of curves, with the Z^{i+1} and the $r_M{}^i$ that produced the error. Study the relationships between them and see if a single functional can be found $Z = f[r]$ that can fit them all to within some merit figure.
5. One might start by trying to develop a functional for a single layer.

Results Using Self-Consistent Iteration

An evaluation was performed using Equation 5 and

$$Z^{new} = R_M^{1/2} - (R_I^{1/2} - Z^{old})$$

with $Z^{old} = 0$ on the first iteration, and the $Q = R_I^{1/2} - Z^{old}$, and an argument $Q\exp(ikx)$ in the integral, and taking the real part of the logarithmic derivative of *n*, and integrating the logarithmic derivative numerically. The process hones in on the low reflectance areas and edges, then after 6 iterations, stagnates. The maximum and minimum indices permitted in the design were 2.3 and 1.5. After the 6th iteration, the maximum index was reduced to 2.23, and then stagnates again at the 13th iteration, Figure 1. The targets were that of a neutral beam splitter with reflectance of 0.5 (50%) from 500-700 nm and 0.01 (1%) to 800 nm and 400 nm.

Rand – you need to go back and redo this using equation 10 for this example. You did not try this. The equation 10 method pre-integrates the index logarithmic derivative, which turns out to be real, so you do not have to take the Re( ) result. You had also been using the MathCad numerical integration routine, which you replaced by a sum, the Equation 10 form.

The procedure could be modified to

$$n^{(i+1)}(z) = \exp\left[\int \frac{R_I^{1/2}(k) - Z^{(i)}}{k}\sin(-kz)dk\right] = n_{NI(I)}n_Z^{(i)}$$

On the first iteration $(i=1)$ $Z^{(1)}=0$ and the second error is computed $Z^{(2)} = R_M{}^{1/2\,(1)} - (R_I{}^{1/2} - Z^{(1)})$ and used in the second iteration $(i=2)$, after the second iteration the third error is computed $Z^{(3)} = R_M{}^{1/2\,(2)} - (R_I{}^{1/2} - Z^{(2)})$ and used in the third iteration $(i=3)$, etc…

On iteration *i*, $Z^{(i)}$ is in the integrand, and

$$Z^{(i)} = \sum_{u=1}^{i-1} R_M^{1/2(u)} - \sum_{u=1}^{i-1} R_I^{1/2}$$

$$n^{(i+1)}(z) = \exp\left[\int \frac{R_I^{1/2}(k) - \left(\sum_{u=1}^{i-1} R_M^{1/2(u)} - \sum_{u=1}^{i-1} R_I^{1/2}\right)}{k} \sin(-kz)dk\right] = \left(n_{NI(I)}\right)^i C^{(i)}$$

Therefore, the $n_{NI(I)}$ need only be computed once and raised to the appropriate i. The $C^{(i)}$ can computed from the running sum of the $R_M{}^{1/2}$ or can be treated as a running product.

$$C^{(i)} = \exp\left[\int \frac{-\left(\sum_{u=1}^{i-1} R_M^{1/2(u)}\right)}{k} \sin(-kz)dk\right] = C^{(i-1)} \exp\left[\int \frac{-R_M^{1/2(i-1)}}{k} \sin(-kz)dk\right]$$

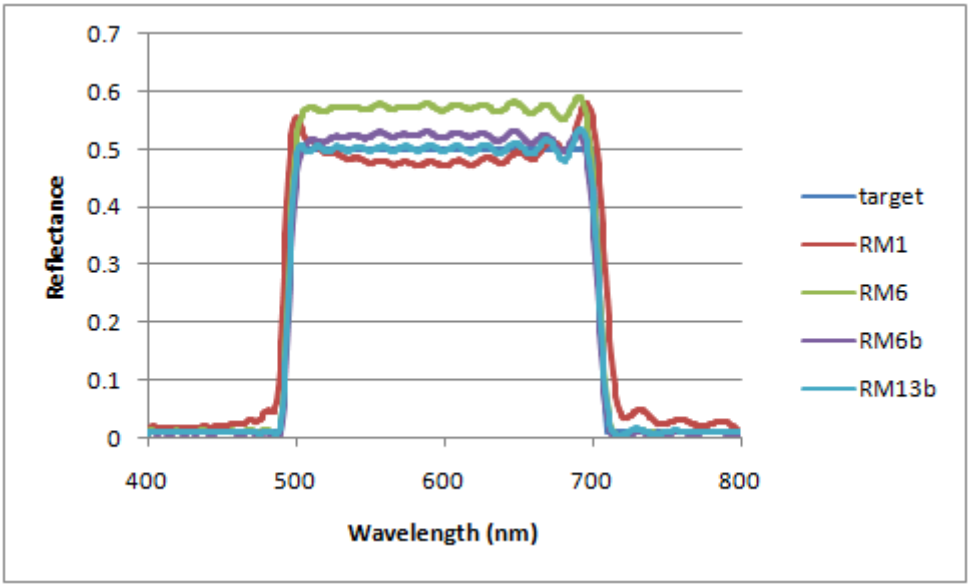

Figure 1. Results of iterating to self-consistency. After 6 iterations, the procedure stagnates. In iteration 6b, the maximum index is reduced to 2.23 from 2.3, and the procedure restagnates at iteration 13b. The spectra are matrix evaluations of the Fourier generated and scaled indices.

Figure 2 shows traditional Q functions $R^{1/2}$ and the "Bovard" $Q = (1/2(T^{-1} - T))^{1/2}$, versus the Q arrived at after iteration to stagnation in 13b, the "Dannenberg" $Q = R^{1/2} - Z^0$, Z^0 being the error in Equation 5.

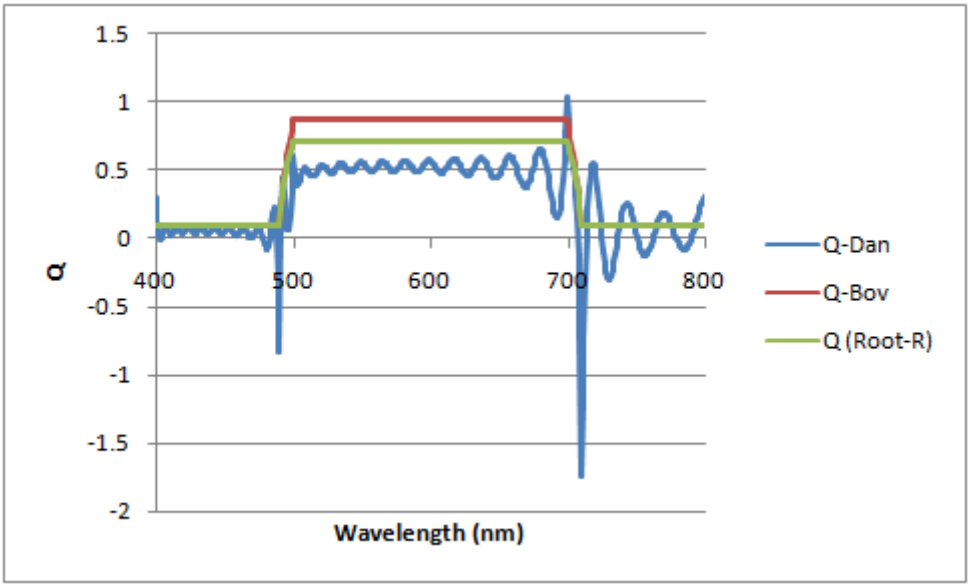

Figure 2. The *Q's* compared. They are all different. The iteratively derived one (for this example) is quite complicated with no clear relation to R_I.

Conclusions.

The iterative procedure seems to work, at least for this example, and the number of adjustable parameters is only three: n_{max}, n_{min}, and the total thickness.

I need to know if this approach is new, or someone else's work has simply been reproduced.

If it is new, ideas for constraining / scaling the index to realistic values, suggestions for improving the procedure, and investigation of its limitations would be welcomed.