The murkiness of CCD materials: Optical modeling of QE, fringing, and absorption in LBNL CCDs

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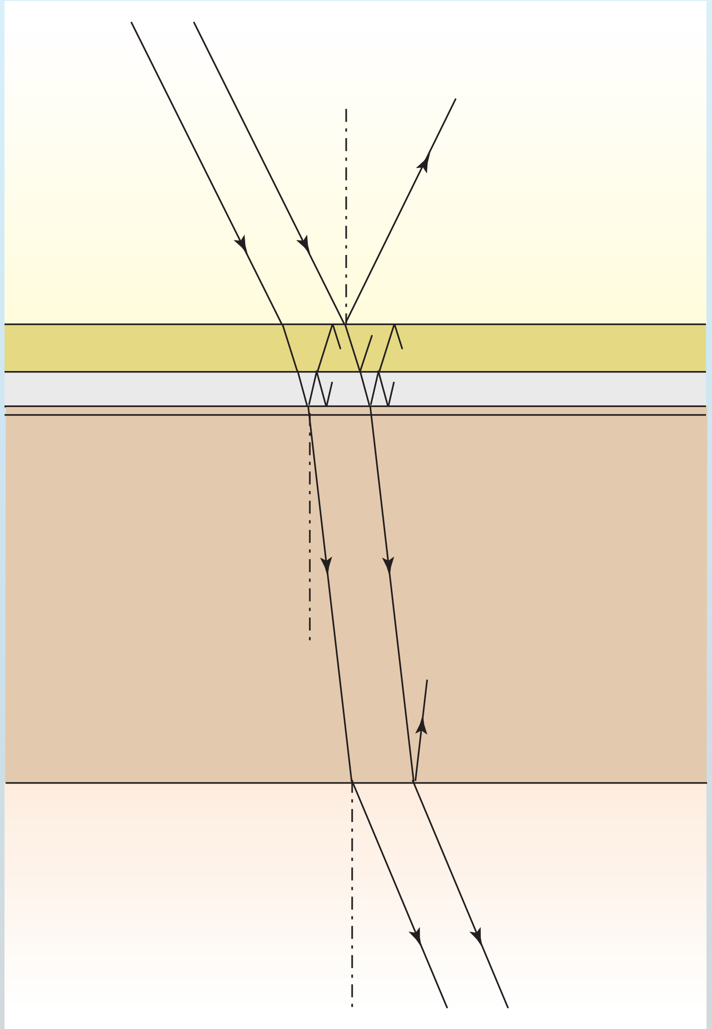
PROLOGUE: At the SDW meeting here in 1999, Jim Beletic asked for a show of hands ---



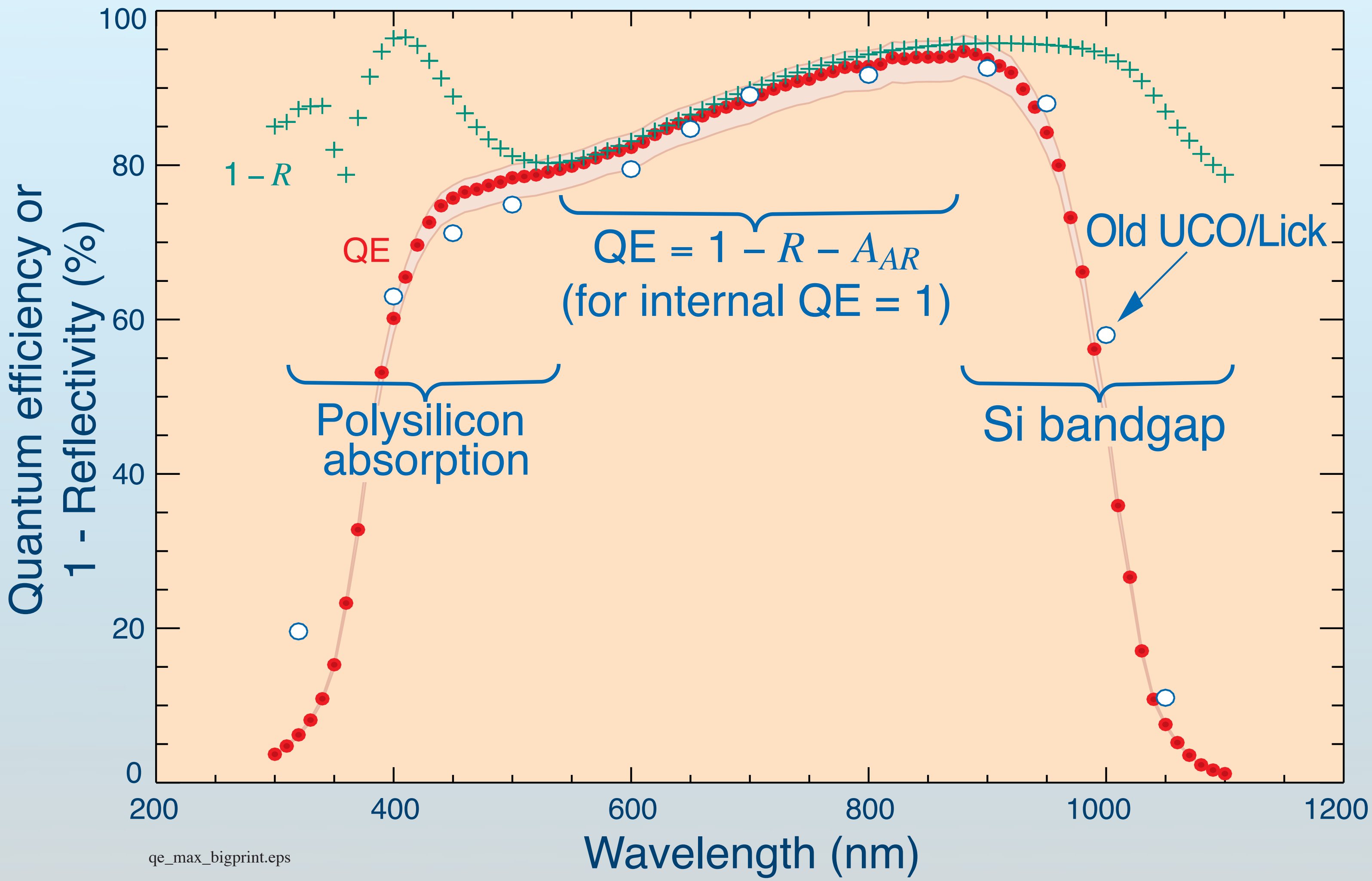
ARproblem_simple_03oct09.eps

"How accurately do you think you can measure the quantum efficiency of a CCD ?"

- 10% ?
- 5% ??
- 1% ??

Successively fewer hands went up

Since then we've learned to measure the reflectivity, which can be done absolutely and easily. (*R* doesn't depend on a standard PD!)
-- and the mid-region can be used to normalize the QE measurements.



(Figure from Maximilion Fabricius' diplomathesis)

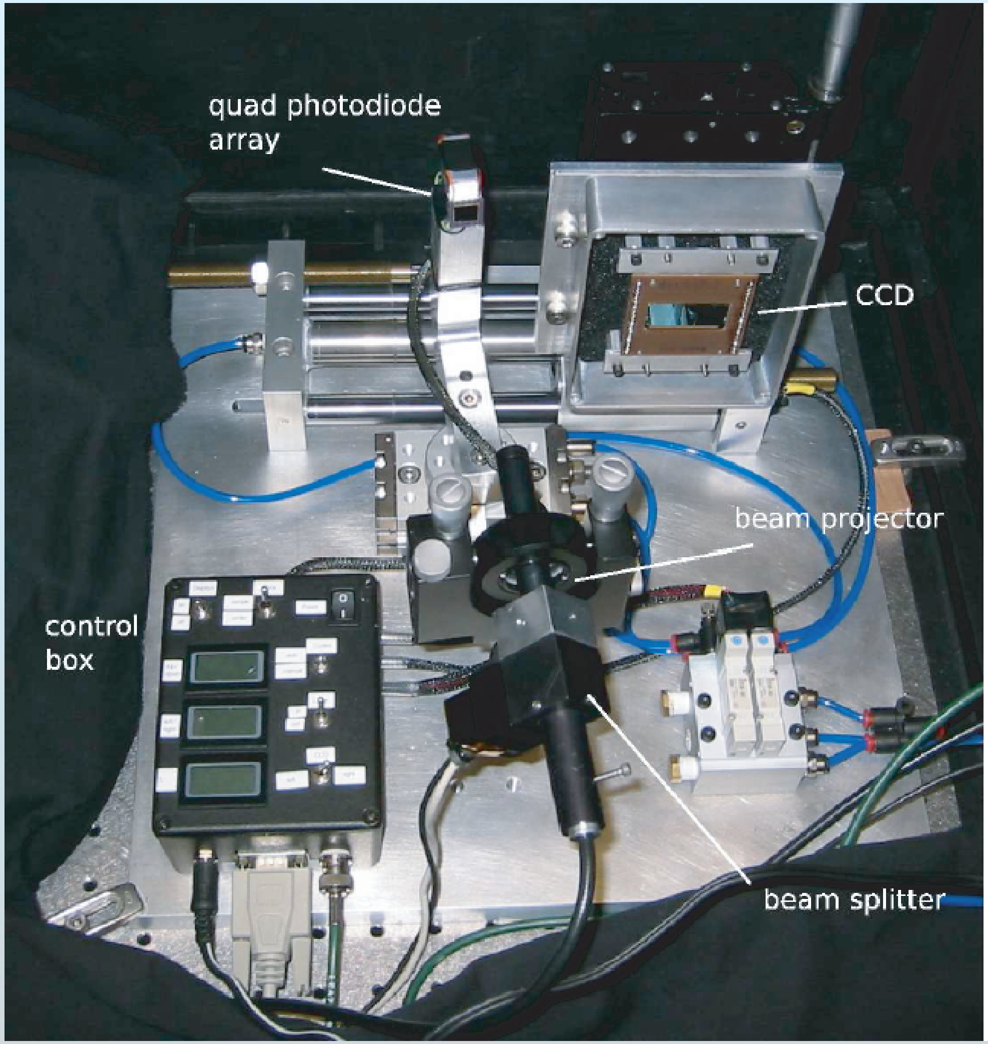
First we built the LBNL QE Machine . . .

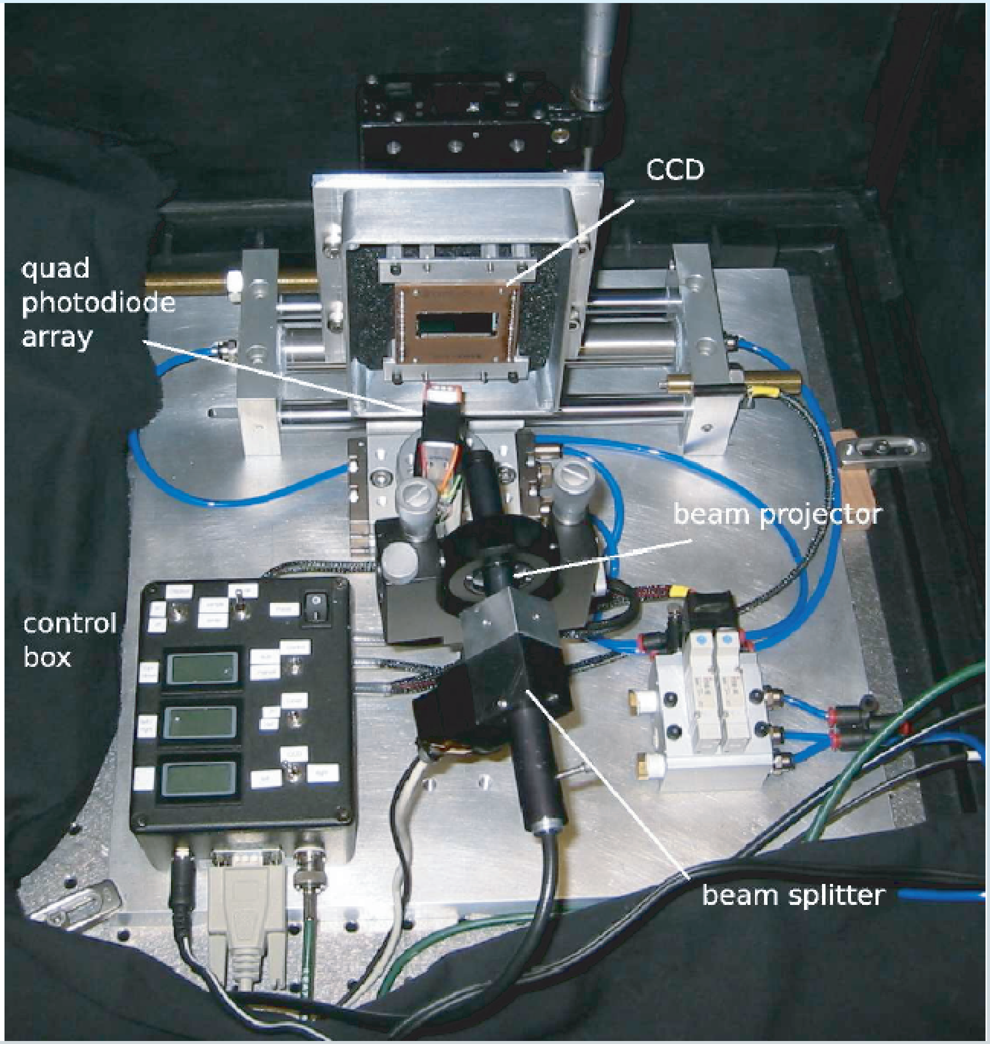
Jens Steckert's diplomathesis; for all practical purposes built by Jens under Armin Karcher's supervision

. . . and then the reflectometer. THIS IS AN ABSOLUTE MEASUREMENT

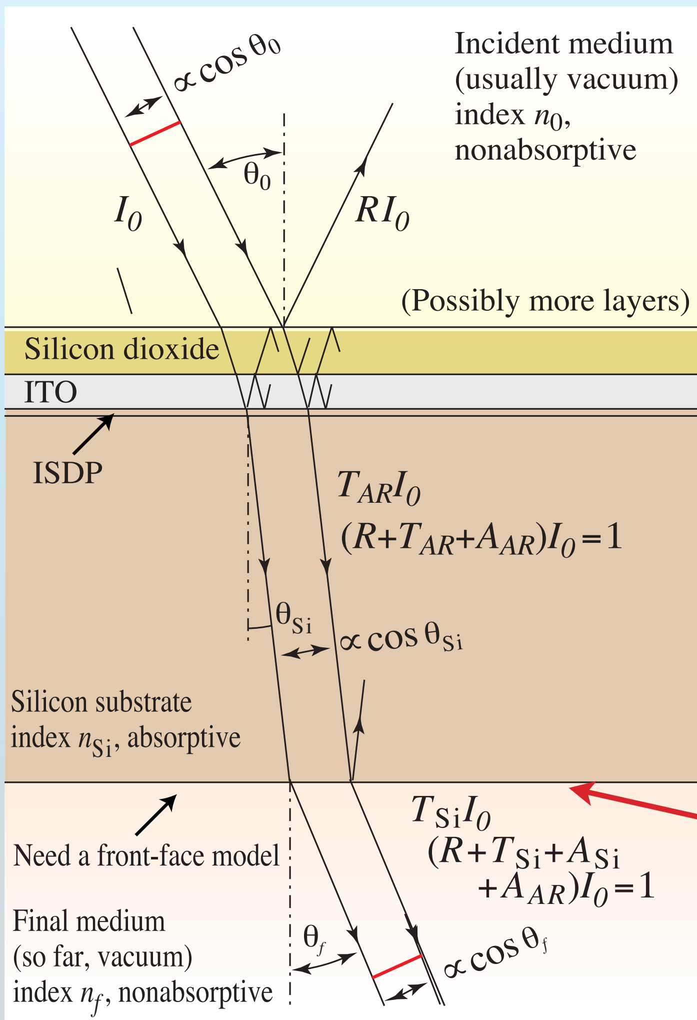
Maximilian Fabricius' diplomathesis; for all practical purposes built by Maximilian under Armin Karcher's supervision

The amazing air-powered action machine!





We've recently attempted to model a coated CCD better: Calculate the reflectivity, transmission, and quantum efficiency of a CCD with (possibly) absorptive coatings.



ARproblem_simple_03oct09.eps

Complication #1 Complication #2

Treat the CCD substrate as a "film," so as to calculate the absorbed fraction (= QE) and fringing

Goals:

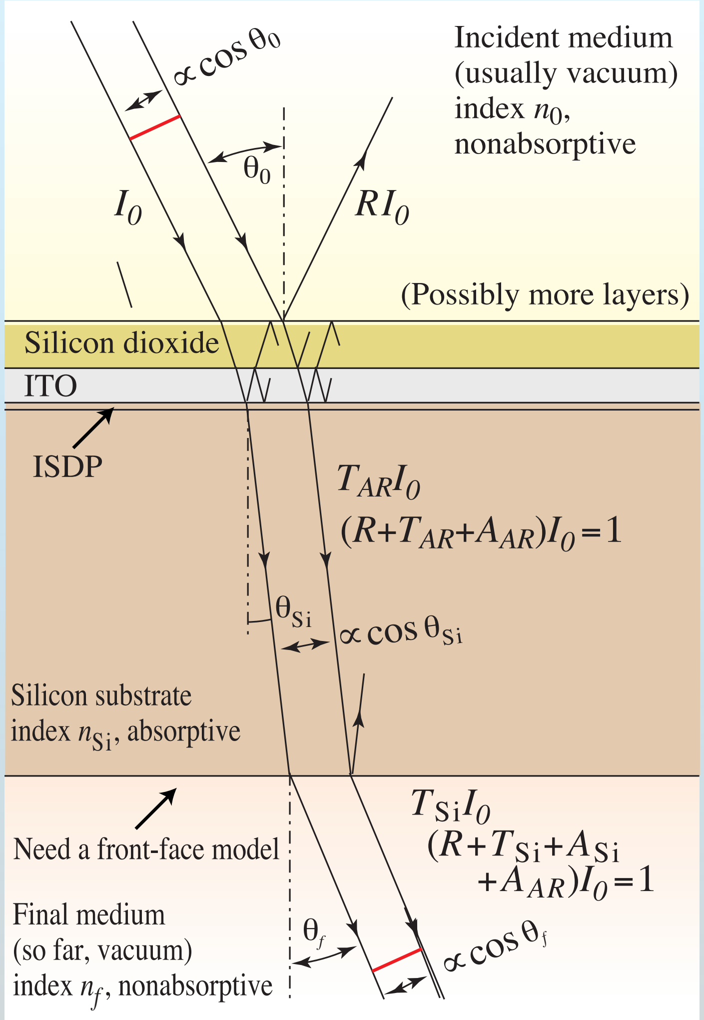
- Find an optimal antireflective coating (maximize QE)
- Understand absorption in the different films
- Sort out reflection from QE and photons lost elsewhere

Complication #3: Front-surface boundary conditions

Apology: Why didn't I just use a commercial package?

In what remains of my 15 min, all I can do is show some results.

I'll specialize to the LBNL CCD, since it has two absorptive layers (besides the substrate). But code is general.



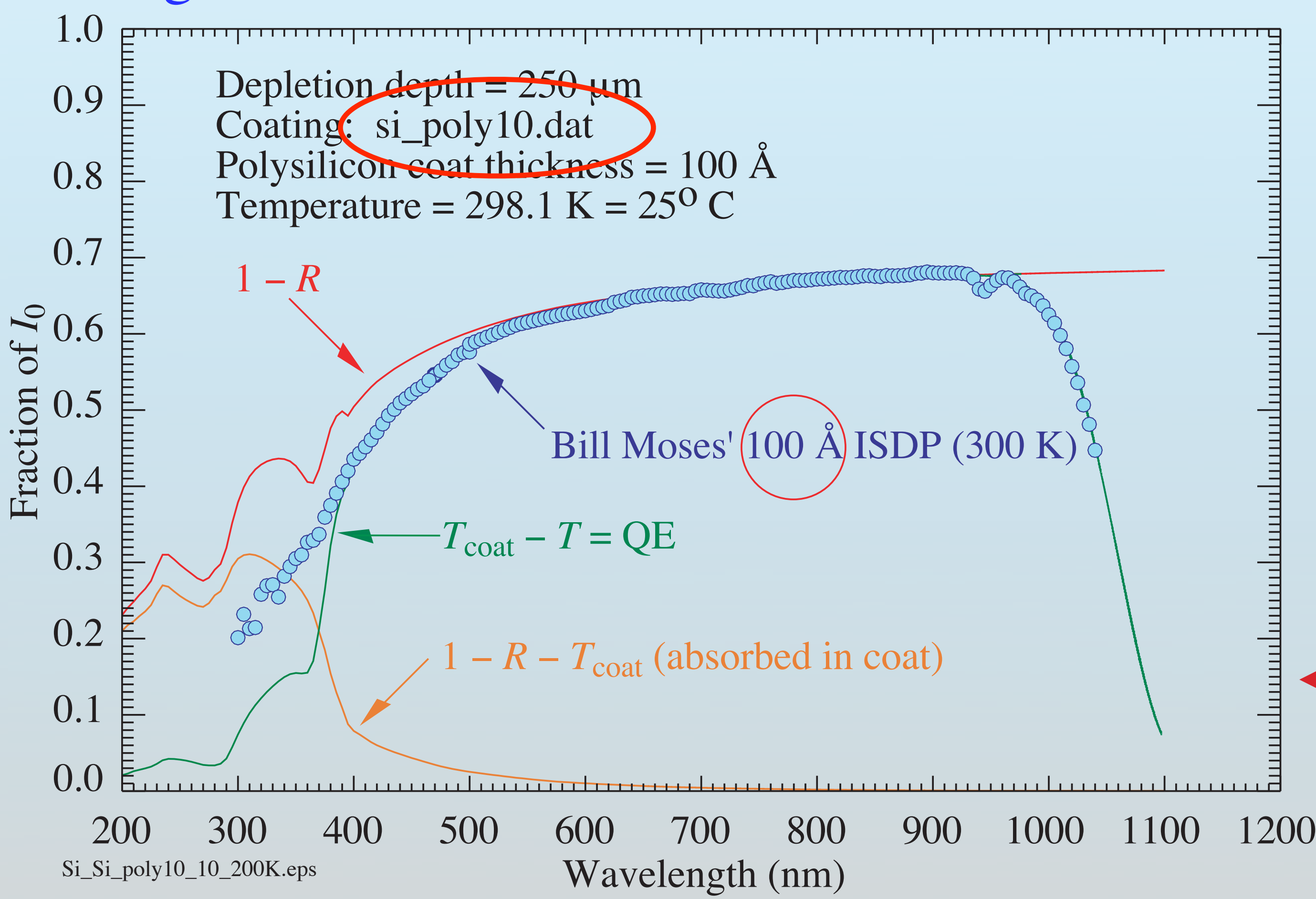
ARproblem_simple_03oct09.eps

One of our problems is the in-situ doped polysilicon (ISDP) backside contact. It was difficult to find the appropriate complex index of refraction.

The index of refraction is complex:

$$n_c = n - ik \qquad (\ell_{\text{abs}} = \lambda/4\pi k)$$

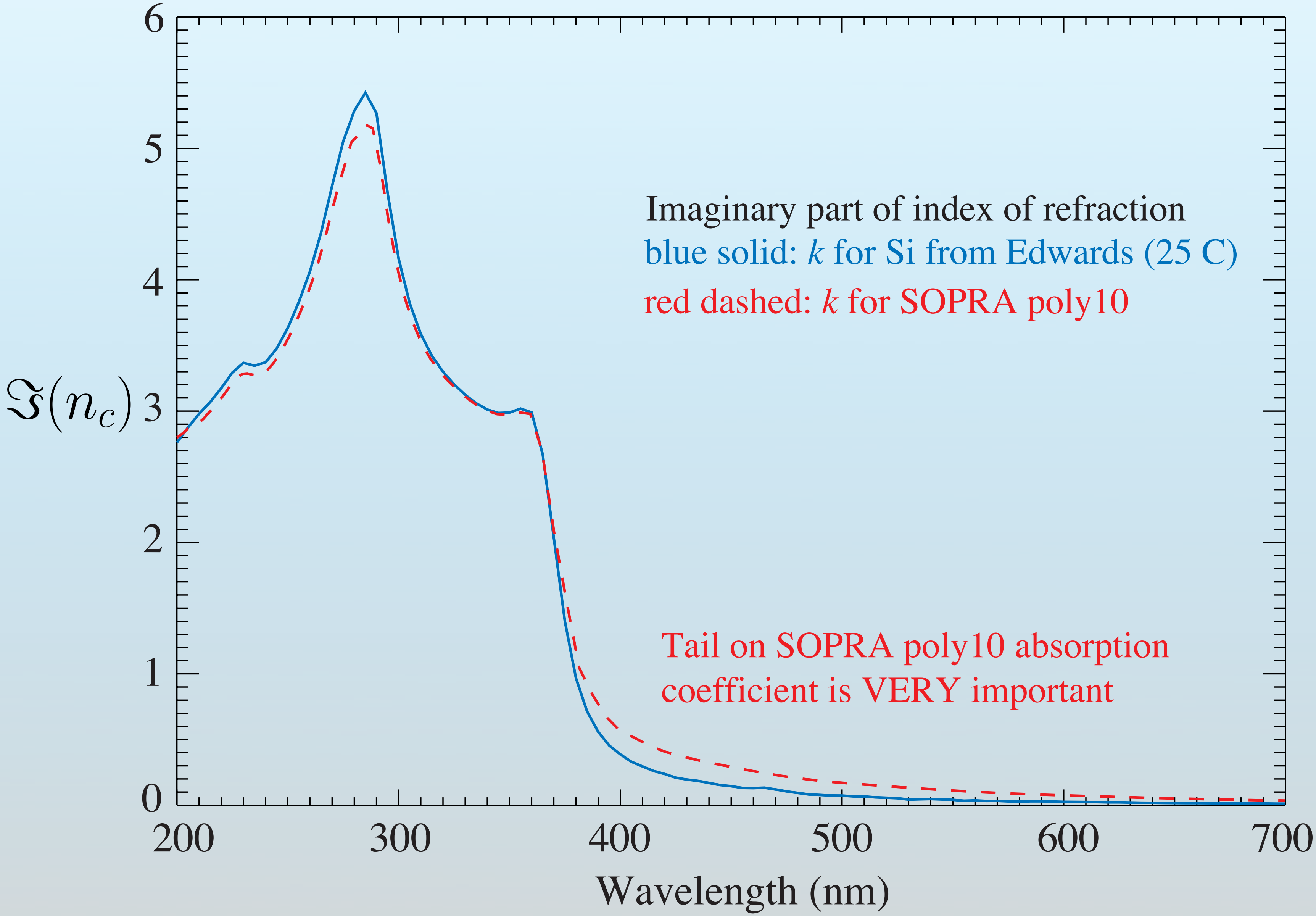
And sometimes hard to find. In addition to the usual literature, the SOPRA database is a gold mine.



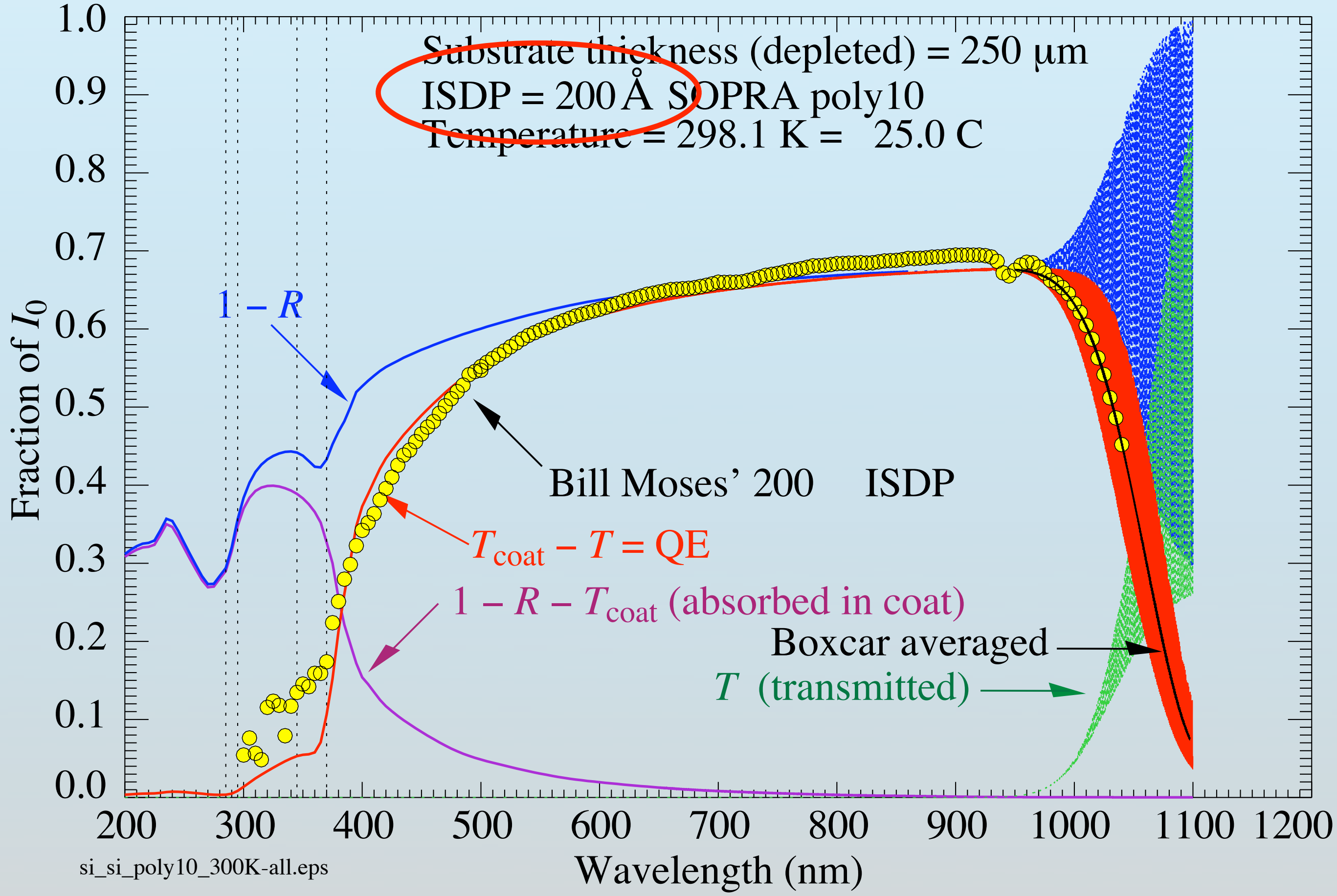
We were lucky enough to have old data from Bill Moses (LBNL), who made a systematic study of the effect of ISDP thickness on photodiode quantum efficiency.

Of the 13 candidate SOPRA tables, "SIPOLY10.NK" provided the best description of the Moses data.

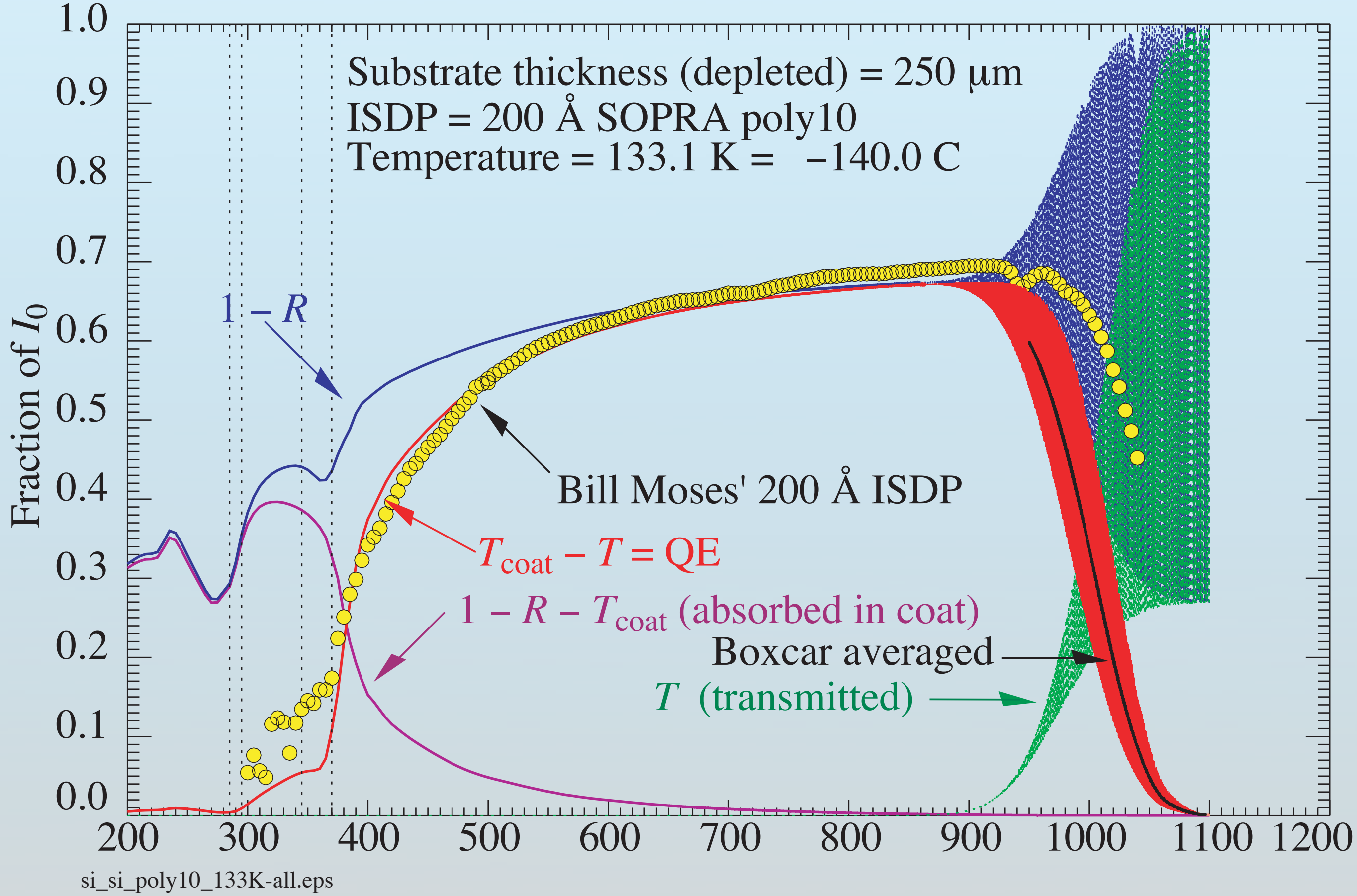
← Naked Si with ISDP coat, on diode at 300K


Imaginary part of index of refraction
blue solid: k for Si from Edwards (25 C)
red dashed: k for SOPRA poly10
Tail on SOPRA poly10 absorption
coefficient is VERY important
$\Im(n_c)$
0
1
2
3
4
5
6
200
300
400
500
600
700
Wavelength (nm)

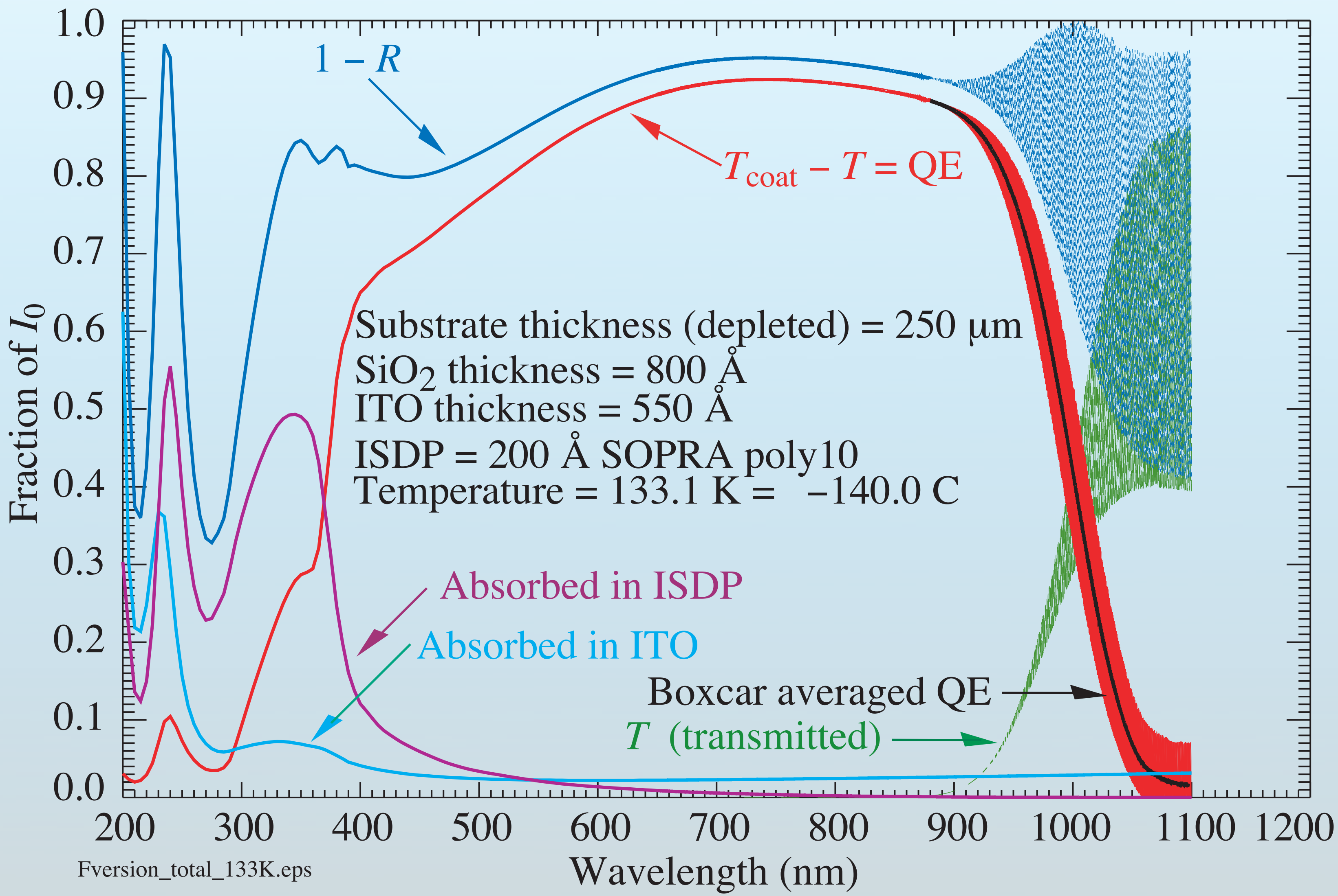
The full calculation looks like this:



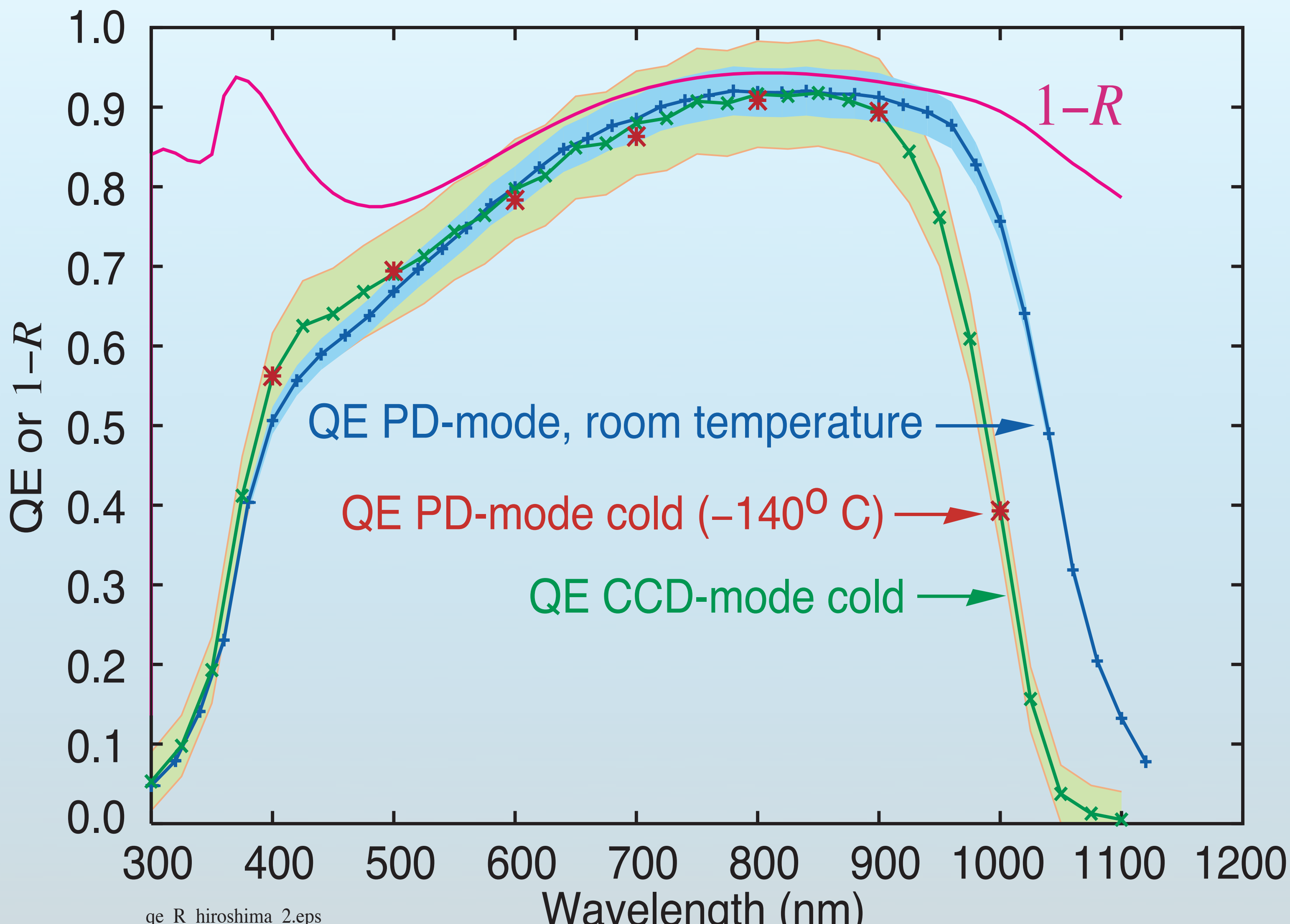
(Side lesson: cooling is hard on the red response)



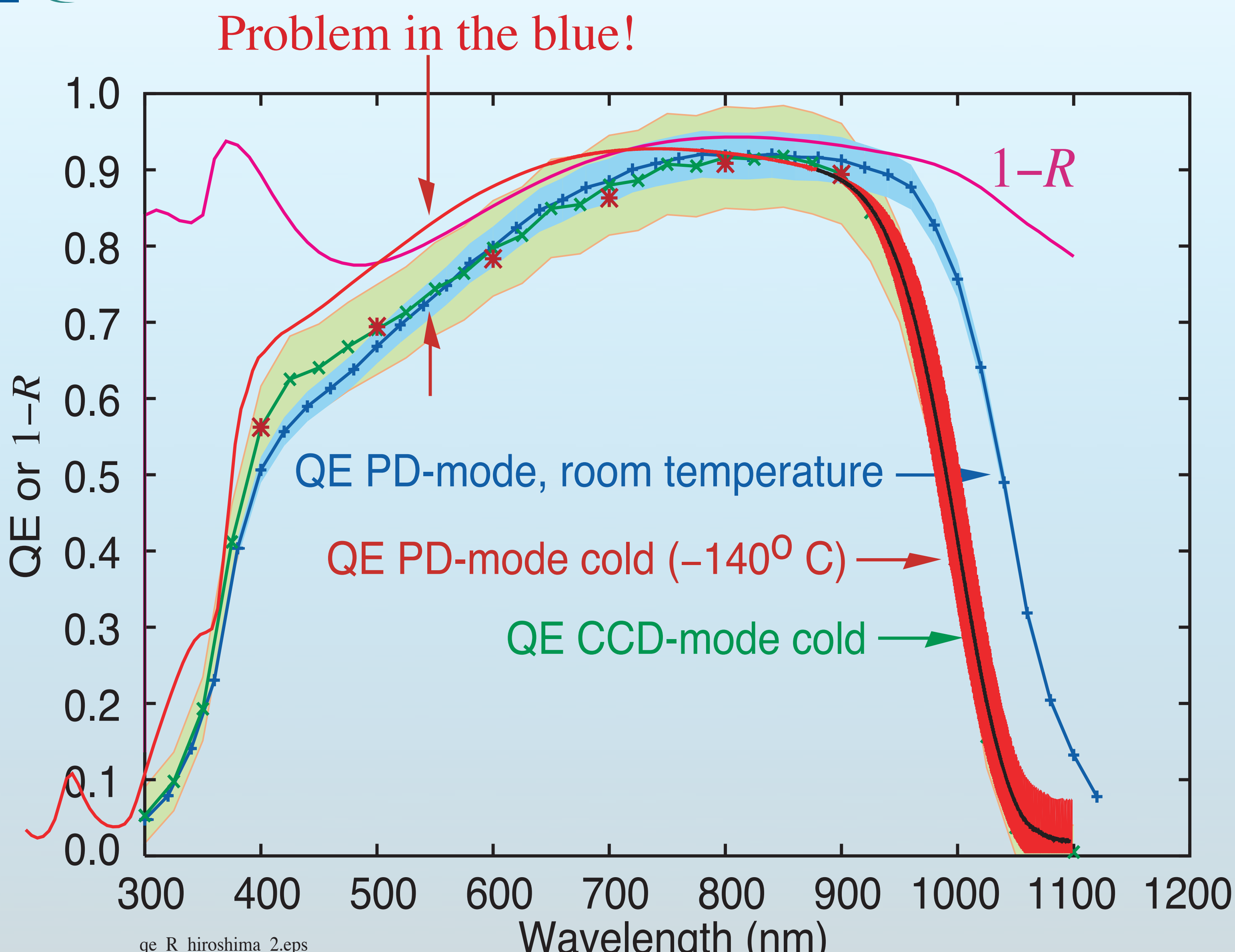
Realistic modeling of the present SNAP CCDs



Difference between 1 - *R* and "central" QE is absorption in the ITO!

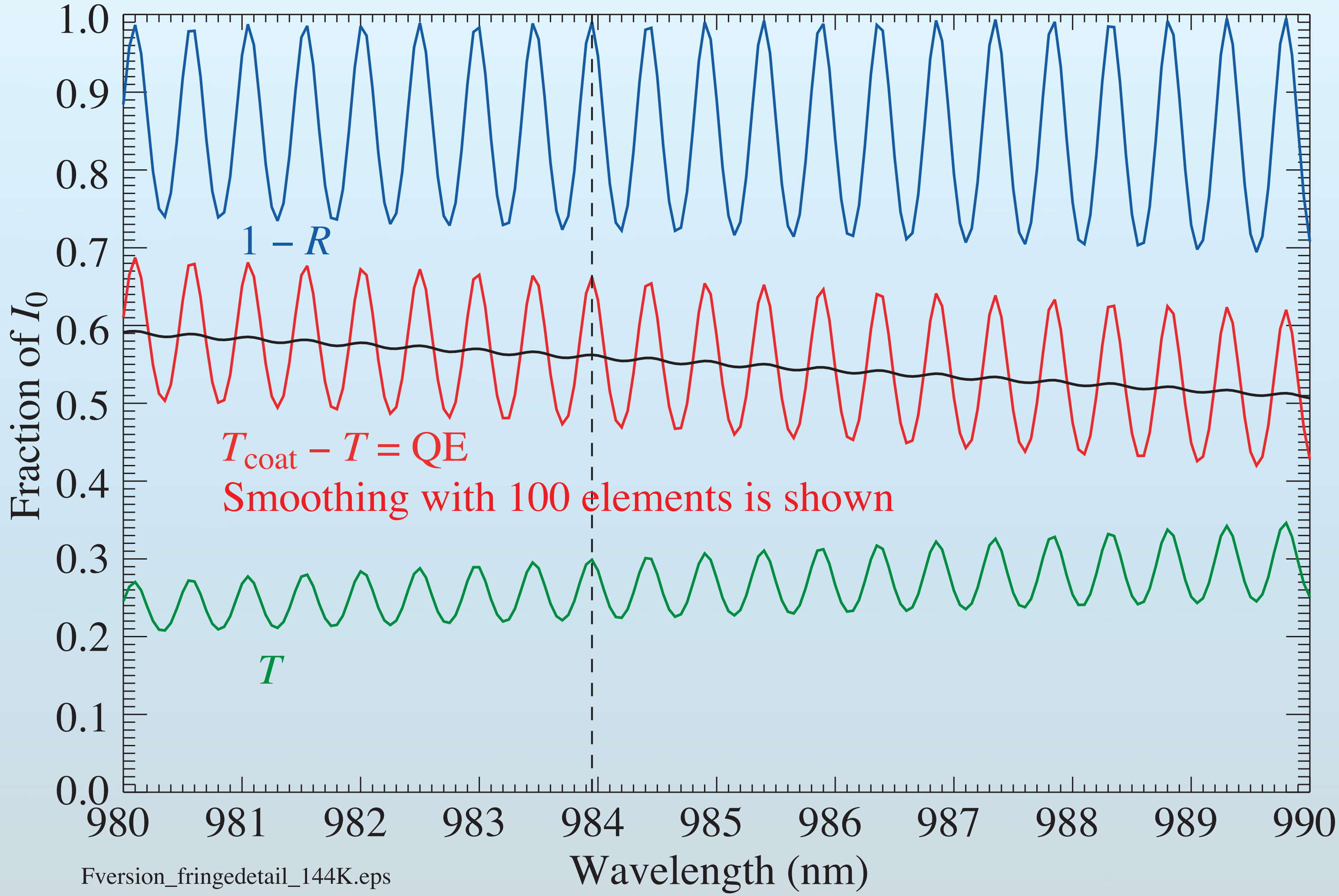


Actual measurements by Maximilion Fabricius



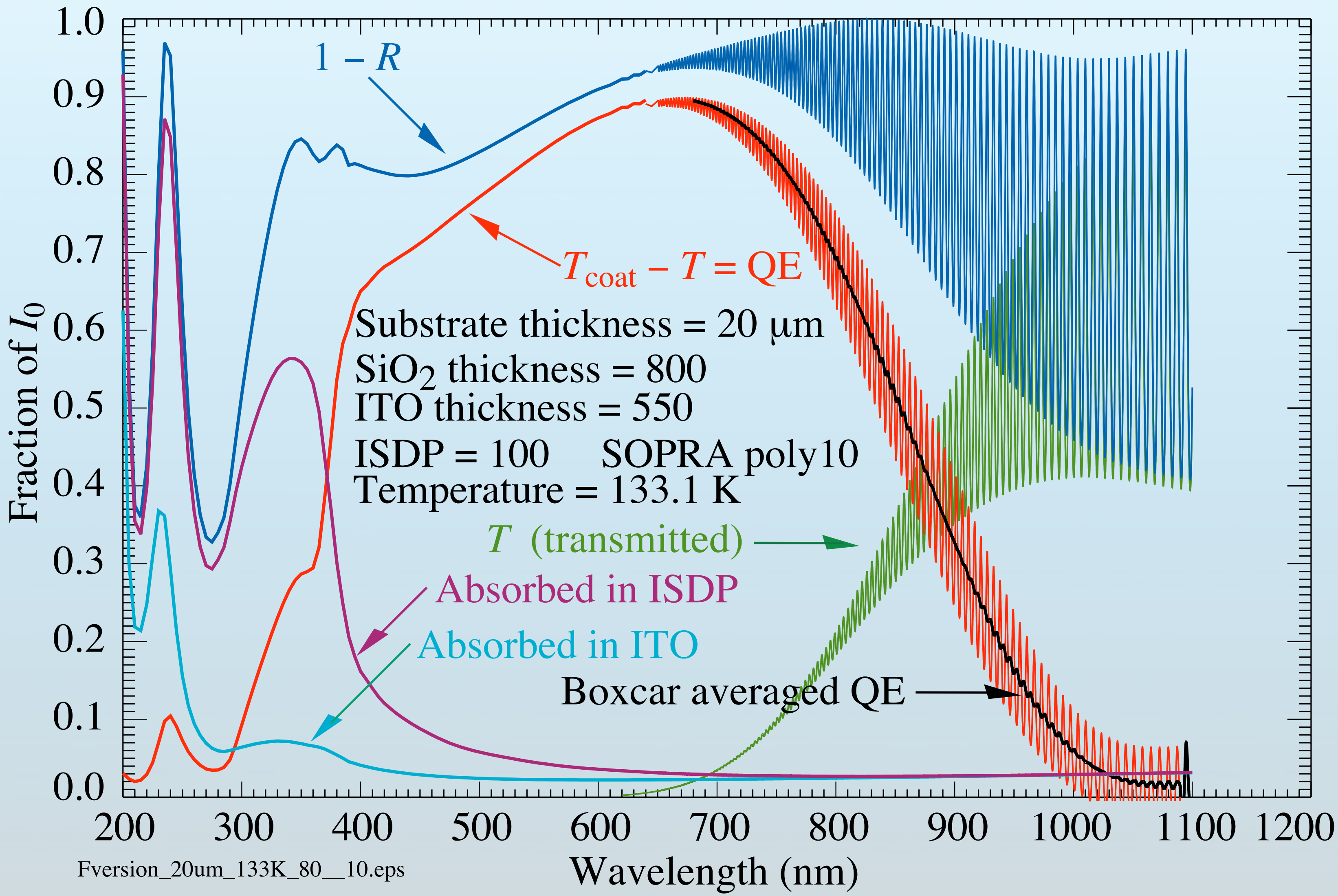
An earlier AR coating recipe had worked fine; here there were also problems with condensation onto the CCD. We take this failure as diagnostic rather than as a problem with the modeling

Fringe region detail



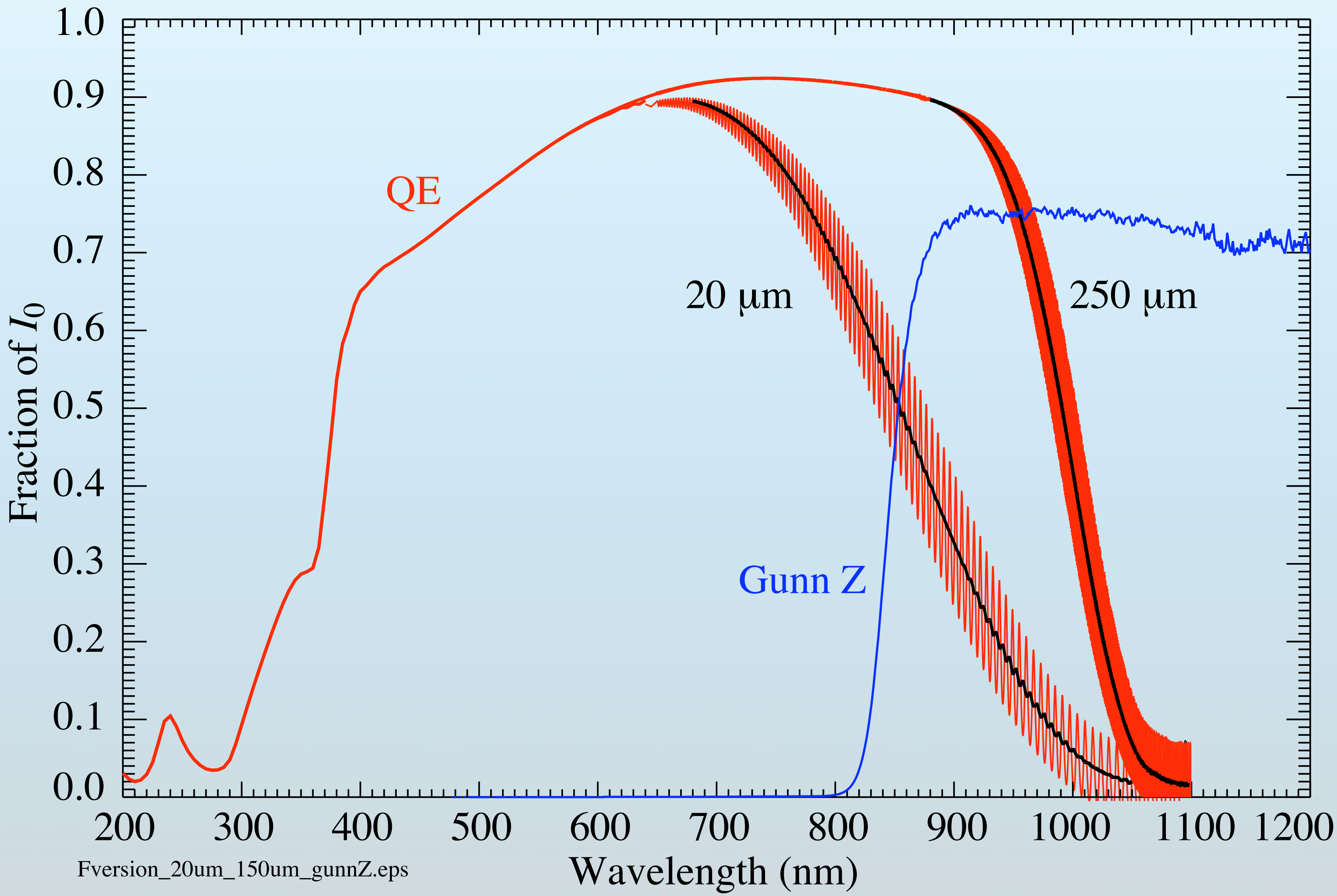
Note "conspiracy" of reflection and transmission to make the fringes less violent!

Calculation for a traditional thinned CCD:



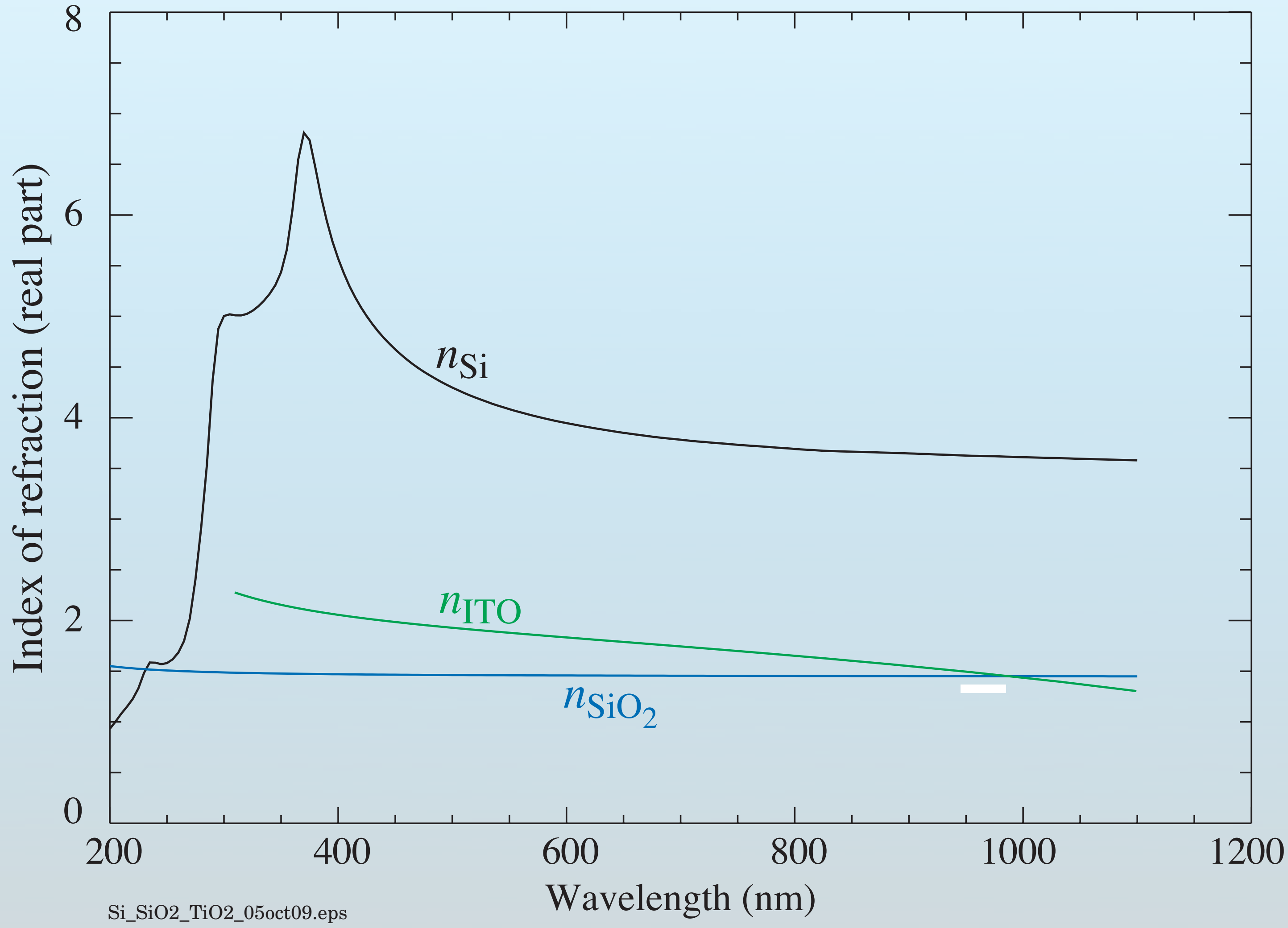
Shows widely spaced fringes extending to below 700 nm.

Thin and thick compared to Gunn Z filter bandpass



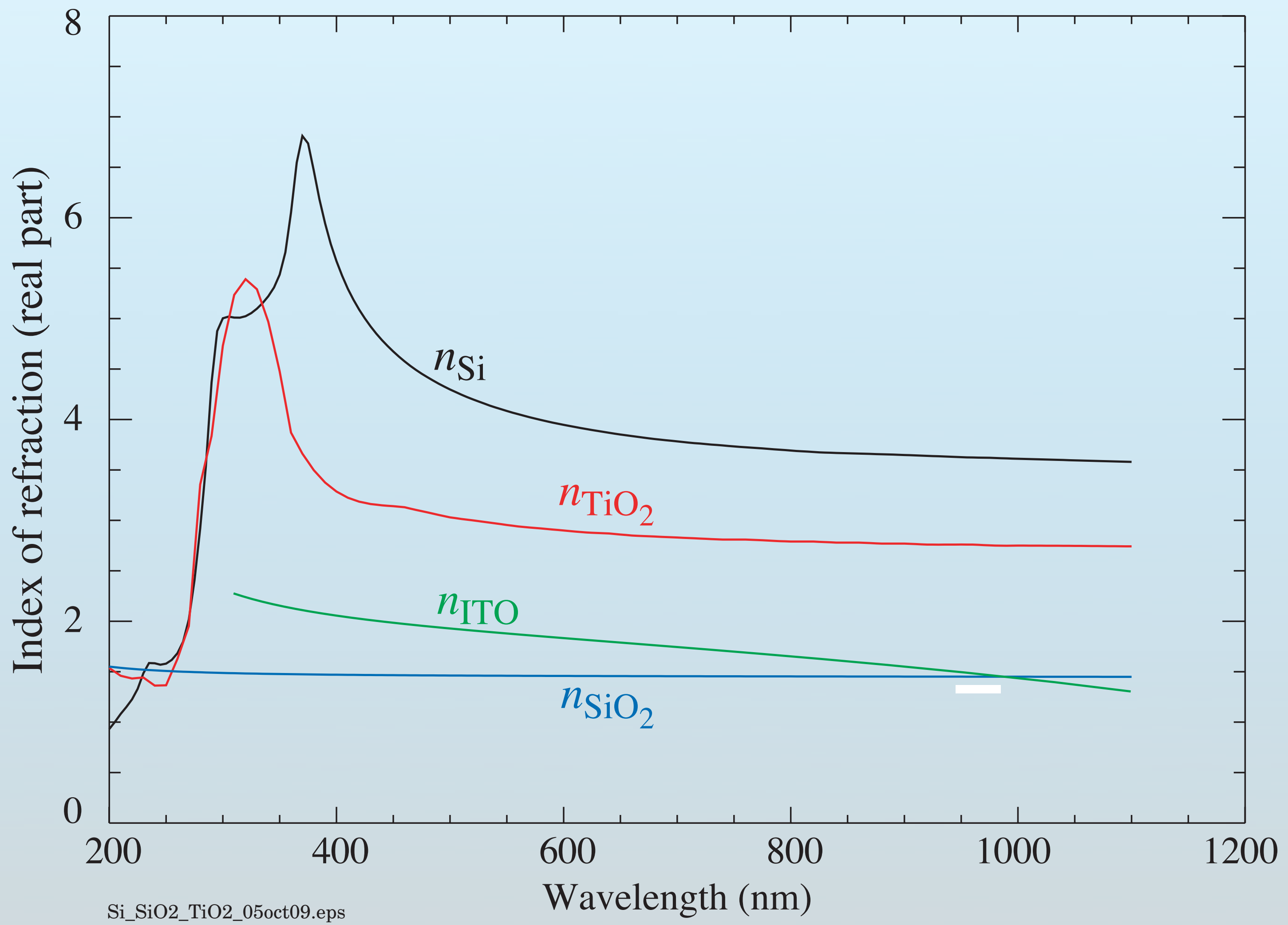
Spacing of fringes: $\delta\lambda = \lambda^2/2nd$

It is surprising at first that the thickness of ITO and Si02 films can be adjusted to get such good response

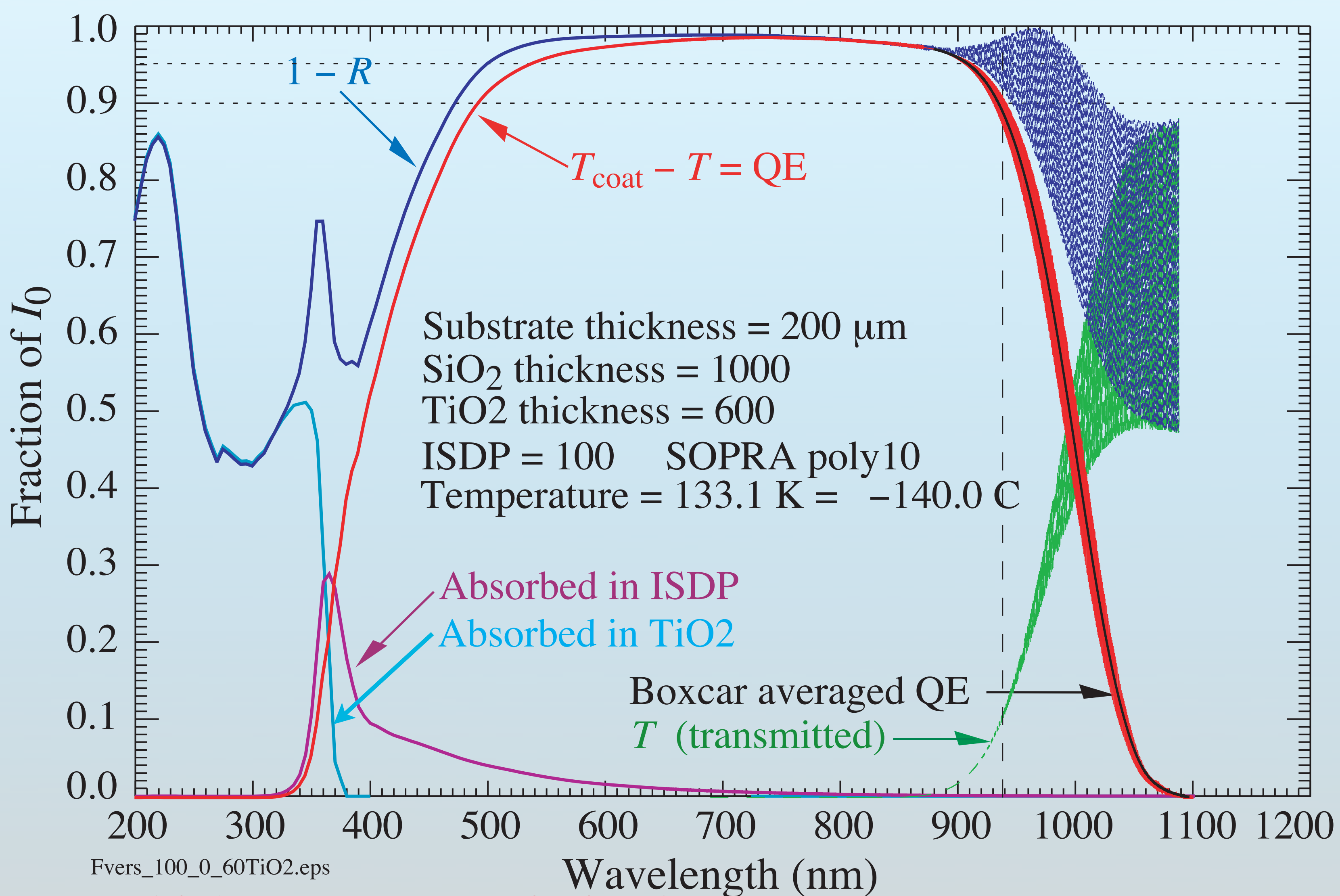


. . . and the ITO index shape doesn't track that of Si very well.

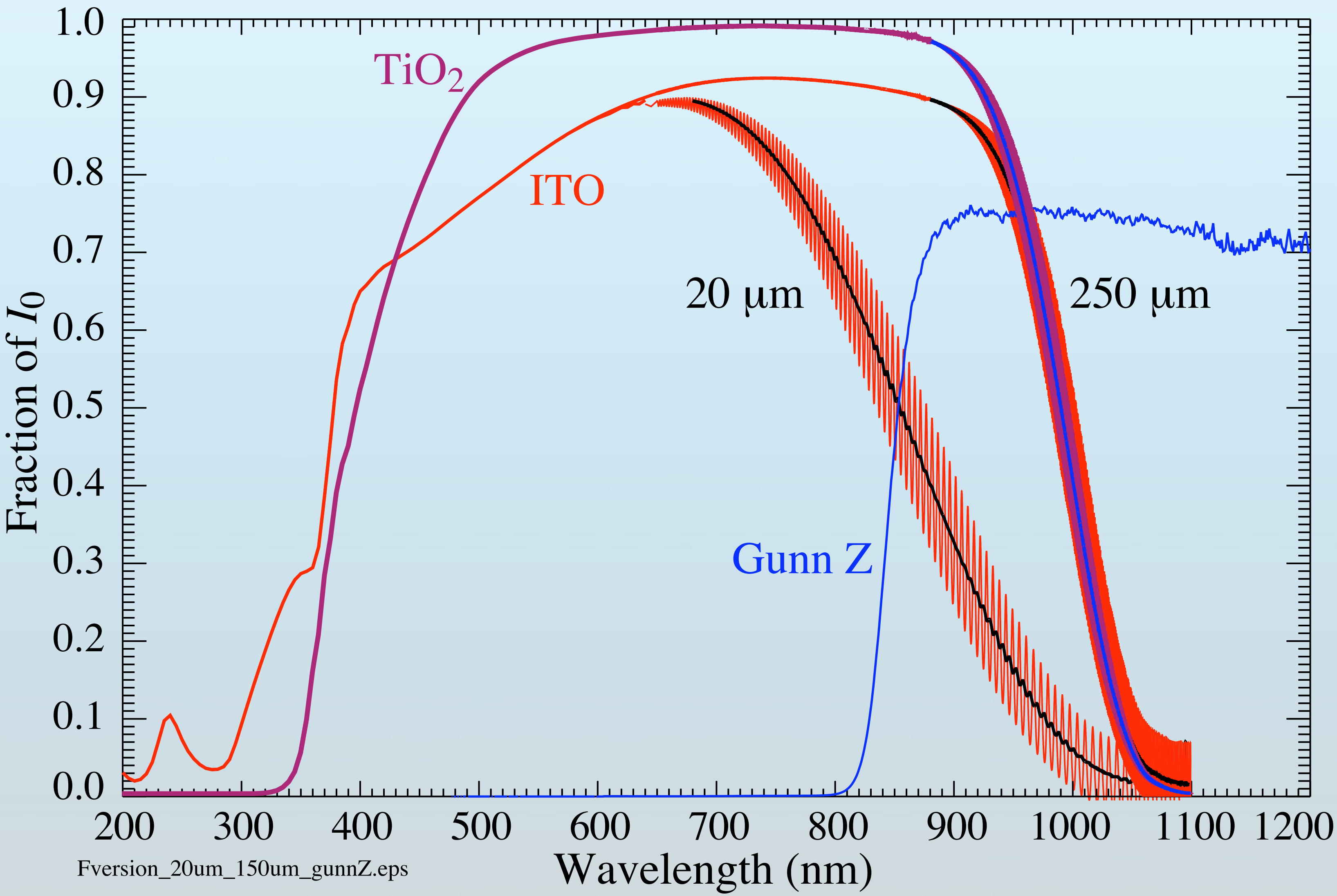
Roger Smith recently told us about the miracle coating, TiO2:



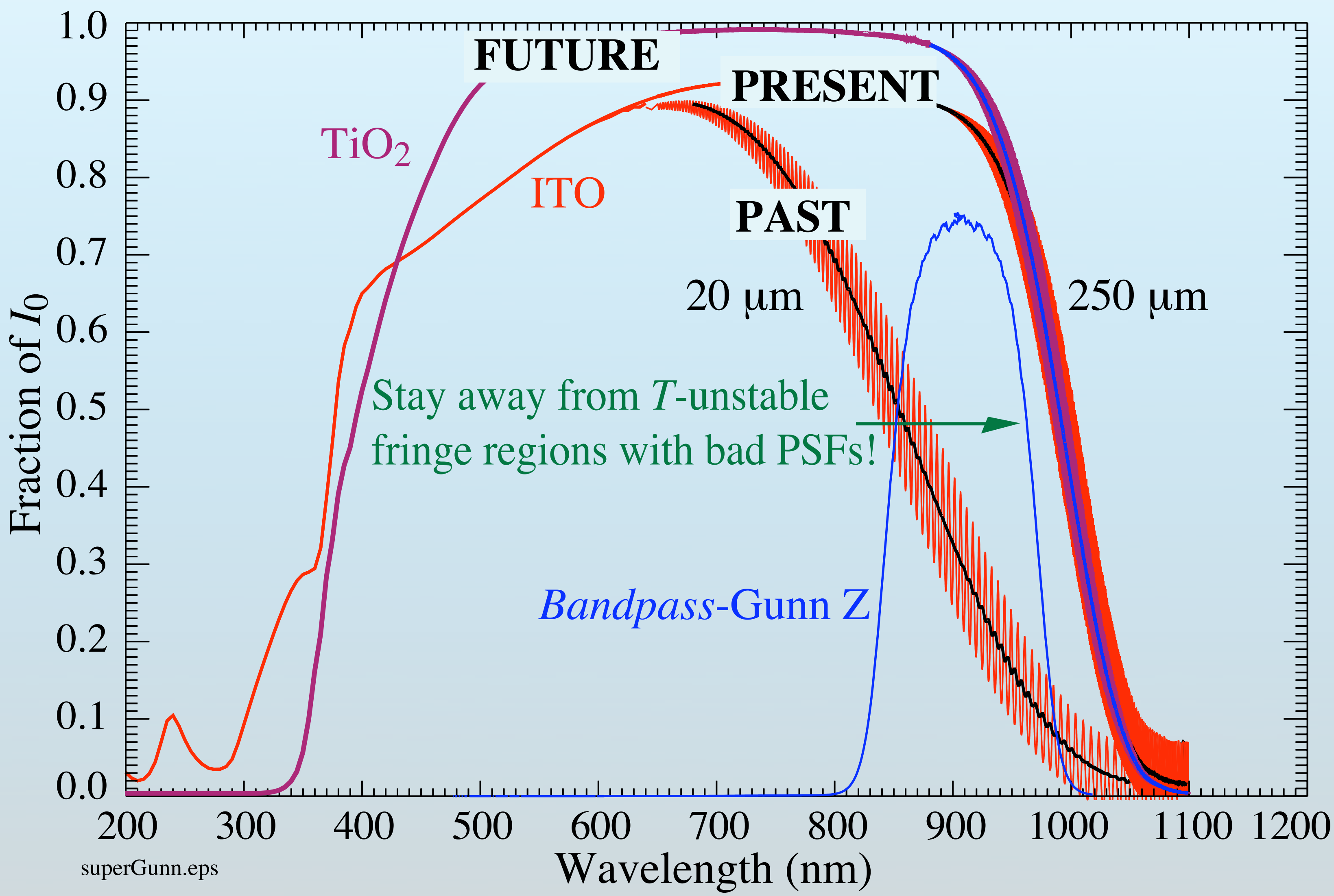
This time the tracking of the Si index is quite respectable!



(Thicknesses not optimized)


1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Fraction of I_0
TiO_2
ITO
20 µm
250 µm
Gunn Z
200
300
400
500
600
700
800
900
1000
1100
1200
Wavelength (nm)
Fversion_20um_150um_gunnZ.eps

. . . and this is a good place to stop!

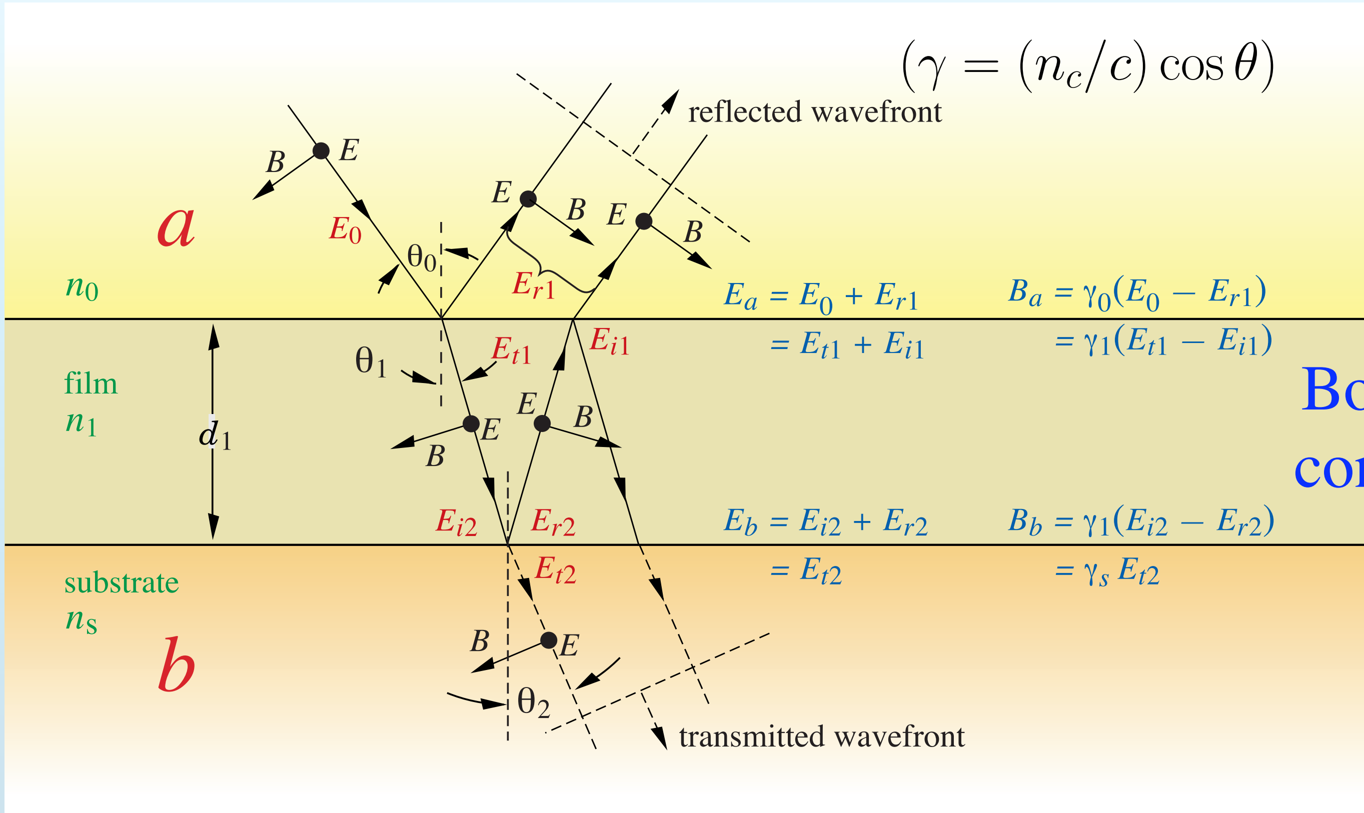


SPARE SLIDES FOLLOW

n_c is the complex index of refraction in a single transit of the *j*th film:

$$n_c = n - ik \qquad (\ell_{\text{abs}} = \lambda/4\pi k)$$

(The sign convention for the absorptive part is not the same in all books-- and has been changed since my previous calculations!)



Boundary conditions

The approach is standard: multiple reflection is taken care of by treating the transmission/reflection at an interface as a boundary condition problem. For normal incidence on a single film, *E* and *B* on entry and exit are related by

$$\begin{pmatrix} E_a \\ B_a \end{pmatrix} = \begin{pmatrix} \cos\delta_1 & \dfrac{i\,\sin\delta_1}{n_{c1}/c} \\ i\,(n_{c1}/c)\sin\delta_1 & \cos\delta_1 \end{pmatrix} \begin{pmatrix} E_b \\ B_b \end{pmatrix} \equiv M_1 \begin{pmatrix} E_b \\ B_b \end{pmatrix}$$

$$\begin{pmatrix} E_a \\ B_a \end{pmatrix} = \begin{pmatrix} \cos\delta_1 & \dfrac{i\,\sin\delta_1}{n_{c1}/c} \\ i\,(n_{c1}/c)\sin\delta_1 & \cos\delta_1 \end{pmatrix} \begin{pmatrix} E_b \\ B_b \end{pmatrix} \equiv \boxed{M_1} \begin{pmatrix} E_b \\ B_b \end{pmatrix}$$

δ_j is the complex phase change in a single transit of the *j*th film:

$$\delta_j = (d_j/\lambda) n_{cj} = \delta_{Rj} + i\delta_{Ij} \quad \leftarrow \text{Note that } \delta_I \text{ is negative!}$$

If there are N films, we just multiply the transfer matrices:

$$\begin{pmatrix} E_a \\ B_a \end{pmatrix} = M_1 M_2 \ldots M_N \begin{pmatrix} E_b \\ B_b \end{pmatrix} \equiv M \begin{pmatrix} E_b \\ B_b \end{pmatrix}$$

So: light with amplitude *I* is incident on film from medium with n_0 (real for initially incident light)

It is reflected (amplitude *r*) and transmitted (amplitude *t*) by the film, emerging into a substrate with index n_s (also generally complex)

$$r = \frac{(n_0 m_{11} + n_0 n_s m_{12}) - (m_{21} + n_s m_{22})}{(n_0 m_{11} + n_0 n_s m_{12}) + (m_{21} + n_s m_{22})} \Longrightarrow R = n_0 \left|r\right|^2$$

$$t = \frac{2n_0}{(n_0 m_{11} + n_0 n_s m_{12}) + (m_{21} + n_s m_{22})} \Longrightarrow T = n_s \left|t\right|^2$$

m is the product of all the relevant transfer matrices

There's one more nuance not usually encountered in normal thin film analysis: What if $e^{-\delta_I}$ overflows the computer? (Remember that it is negative, and for blue light in the substrate it can be hundreds of thousands)

$$
\begin{aligned}
\cos\delta &= \cos\delta_R \cos i\delta_I - \sin\delta_R \sin i\delta_I \\
&= \cos\delta_R \cosh\delta_I - i \sin\delta_R \sinh\delta_I \\
&= e^{-\delta_I} \tfrac{1}{2} \left[\cos\delta_R \left(1 + e^{2\delta_I}\right) + i \sin\delta_R \left(1 - e^{2\delta_I}\right)\right] \\
&\equiv e^{-\delta_I} \, \mathrm{Fcos}\left(\delta_R, \delta_I\right)
\end{aligned}
$$

And similarly for $\sin\delta$. So replace δ_{Ij} with -10 for $\delta_{Ij} < -10$ and write factored matrices:

$$\mathcal{M}_j \equiv e^{-\delta_{Ij}} \mathcal{M}_j^F$$

Then

$$r = \frac{(n_0 m_{11}^F + n_0 n_s m_{12}^F) - (m_{21}^F + n_s m_{22}^F)}{(n_0 m_{11}^F + n_0 n_s m_{12}^F) + (m_{21}^F + n_s m_{22}^F)}$$

← Absorptive substrate doesn't affect reflection

$$t = \frac{2 n_0 \exp\left(\sum \delta_{Ij}\right)}{(n_0 m_{11}^F + n_0 n_s m_{12}^F) + (m_{21}^F + n_s m_{22}^F)}$$

← If there's a really absorptive substrate, no transmission

For wavelengths less than about 900 nm, there IS no reflection from the “front” surface!

And there is very little reflection from the ITO-ISDP interface at any wavelength (zero for > 400 nm, 0.07 at 350 nm).

$$\begin{pmatrix} E_a \\ B_a \end{pmatrix} = M_{\mathrm{AR}} \begin{pmatrix} E_{b\,\mathrm{AR}} \\ B_{b\,\mathrm{AR}} \end{pmatrix}$$

Added later:
Maybe that should be 0.07%

So:

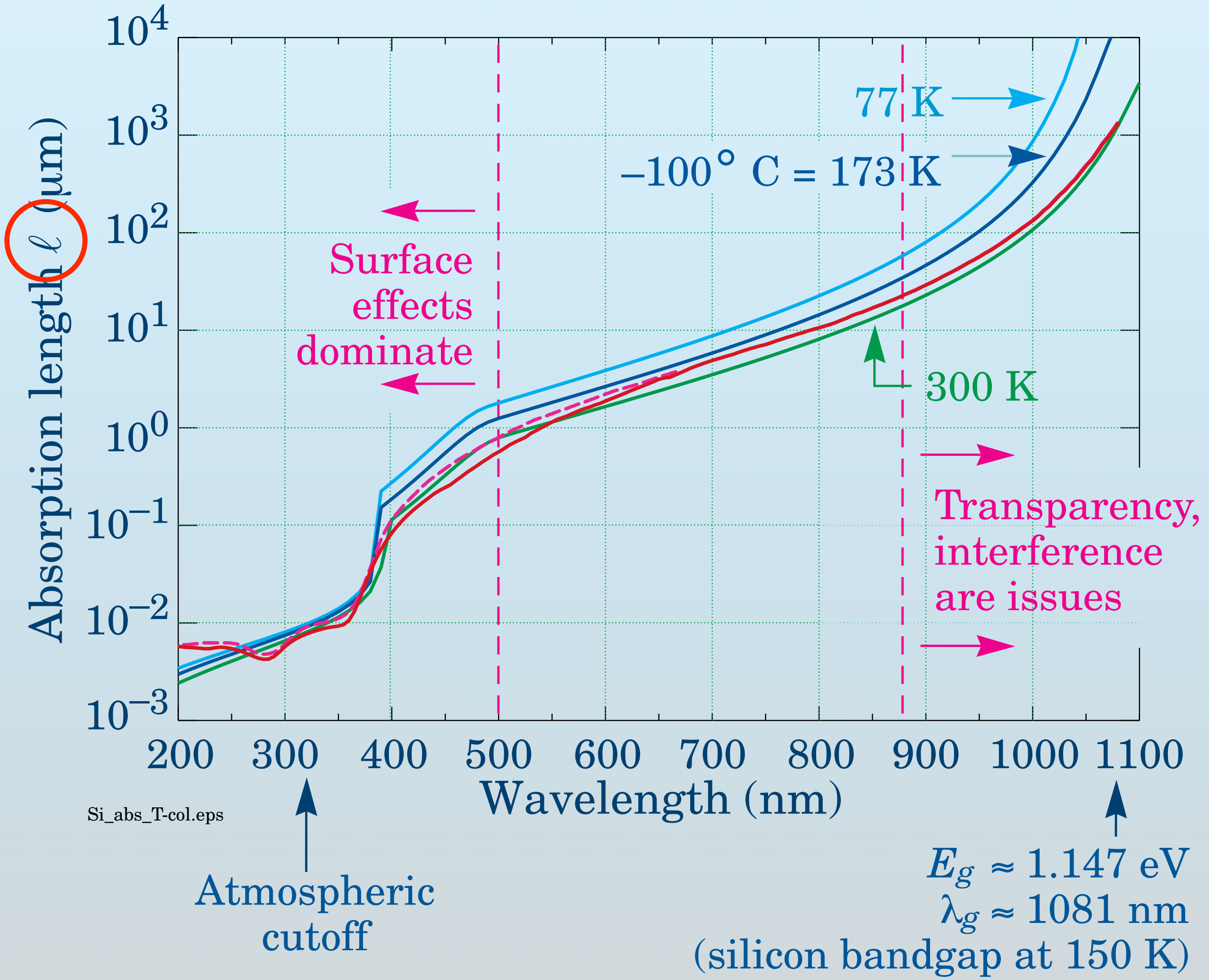
1. Let $M_{AR} = M_{\mathrm{SiO_2}} M_{ITO}$; calculate *R* and *T* with a Si substrate.

2. Let $M_{AR} = M_{\mathrm{SiO_2}} M_{ITO} M_{ISDP}$; calculate *R* and *T* with a Si substrate.

3. For the complete CCD, calculate *R* and *T* with an AIR substrate.

$\Longrightarrow$ Subtract appropriately to find absorption in ITO, ISDP, and Si (=QE)

$$n_c = n - ik, \qquad k = \lambda/4\pi\ell$$



Red is from Janesick and tabulated *n* and *k* for silicon. Note inflections at short wavelengths.

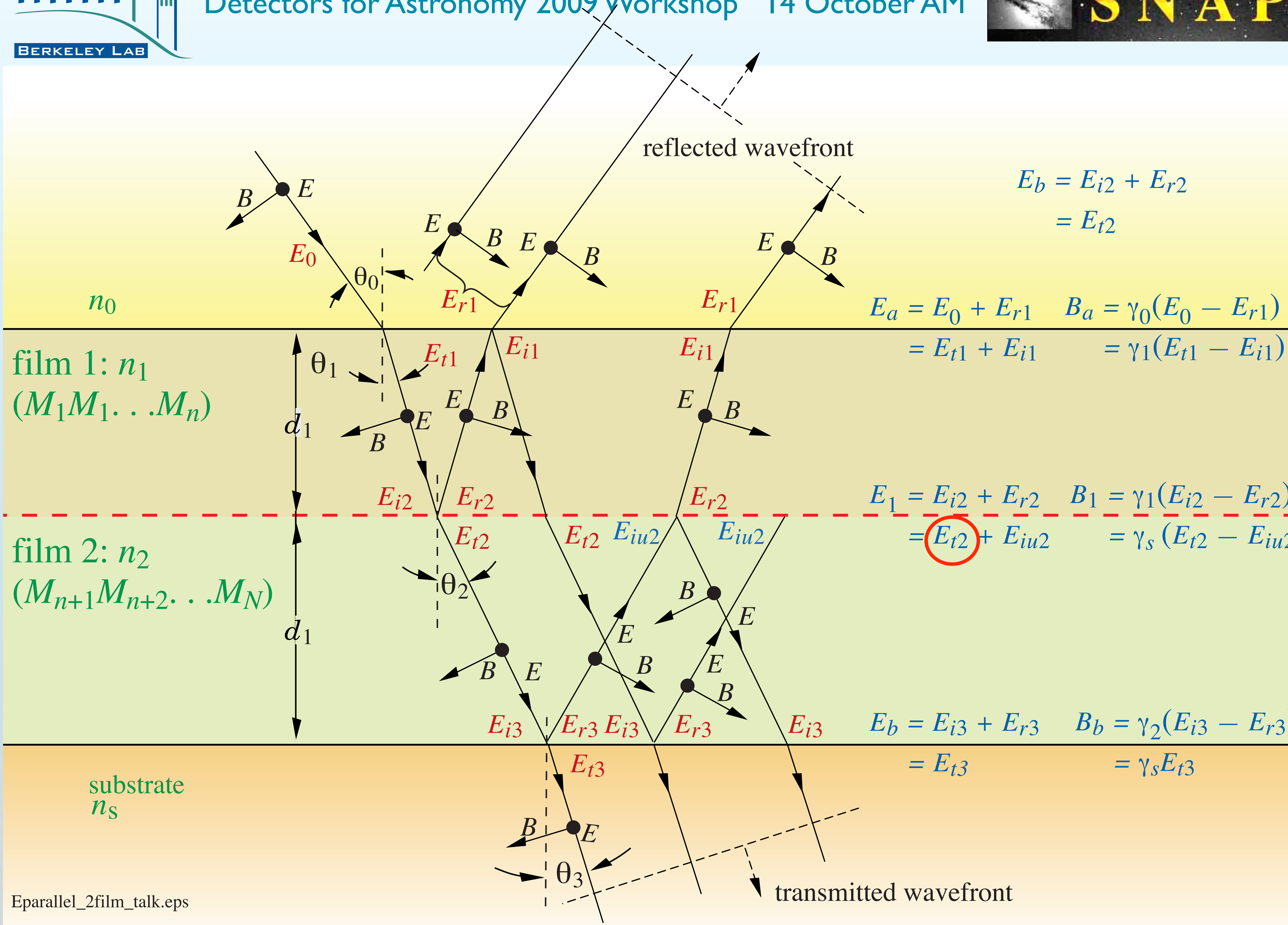
T dependent curves from Rajkanan, Singh, and Shewchun. Note monotonic behavior, unlike the tabulated case.

So in contrast to previous modeling:

☺ Results at the blue end (< 500 nm) can be trusted somewhat, since the Si + ISDP (SOPRA poly10) results agree with Bill Moses' measurements (diodes)

☺ Absorption in the ITO and ISDP are clearly separated, at least for wavelengths < 900 nm

☹ There is a formal problem in the separation, especially important at wavelengths > 900 nm. Before proceeding, I would like to try to solve that problem


reflected wavefront
$E_b = E_{i2} + E_{r2}$
$= E_{t2}$
n_0
E_0
θ_0
E_{r1}
E_{r1}
$E_a = E_0 + E_{r1}$
$= E_{t1} + E_{i1}$
$B_a = \gamma_0(E_0 - E_{r1})$
$= \gamma_1(E_{t1} - E_{i1})$
film 1: n_1
$(M_1 M_1 \ldots M_n)$
θ_1
E_{t1}
E_{i1}
E_{i1}
d_1
E_{i2}
E_{r2}
E_{r2}
$E_1 = E_{i2} + E_{r2}$
$= E_{t2} + E_{iu2}$
$B_1 = \gamma_1(E_{i2} - E_{r2})$
$= \gamma_s(E_{t2} - E_{iu2})$
film 2: n_2
$(M_{n+1} M_{n+2} \ldots M_N)$
E_{t2}
E_{t2}
E_{iu2}
E_{iu2}
θ_2
d_1
E_{i3}
E_{r3}
E_{i3}
E_{r3}
E_{i3}
$E_b = E_{i3} + E_{r3}$
$= E_{t3}$
$B_b = \gamma_2(E_{i3} - E_{r3})$
$= \gamma_s E_{t3}$
substrate
n_S
E_{t3}
θ_3
transmitted wavefront
Eparallel_2film_talk.eps

$(\gamma = (n_c/c)\cos\theta)$

The phase shift \delta as the light goes through the film once is nc(2pid/\lambda)
nc = n - i k

Given all those complex indices, I wanted to sort through Maxwell's equations to see how it all worked.

Example: the intensity *I*, the magnitude of the Pointing vector, is

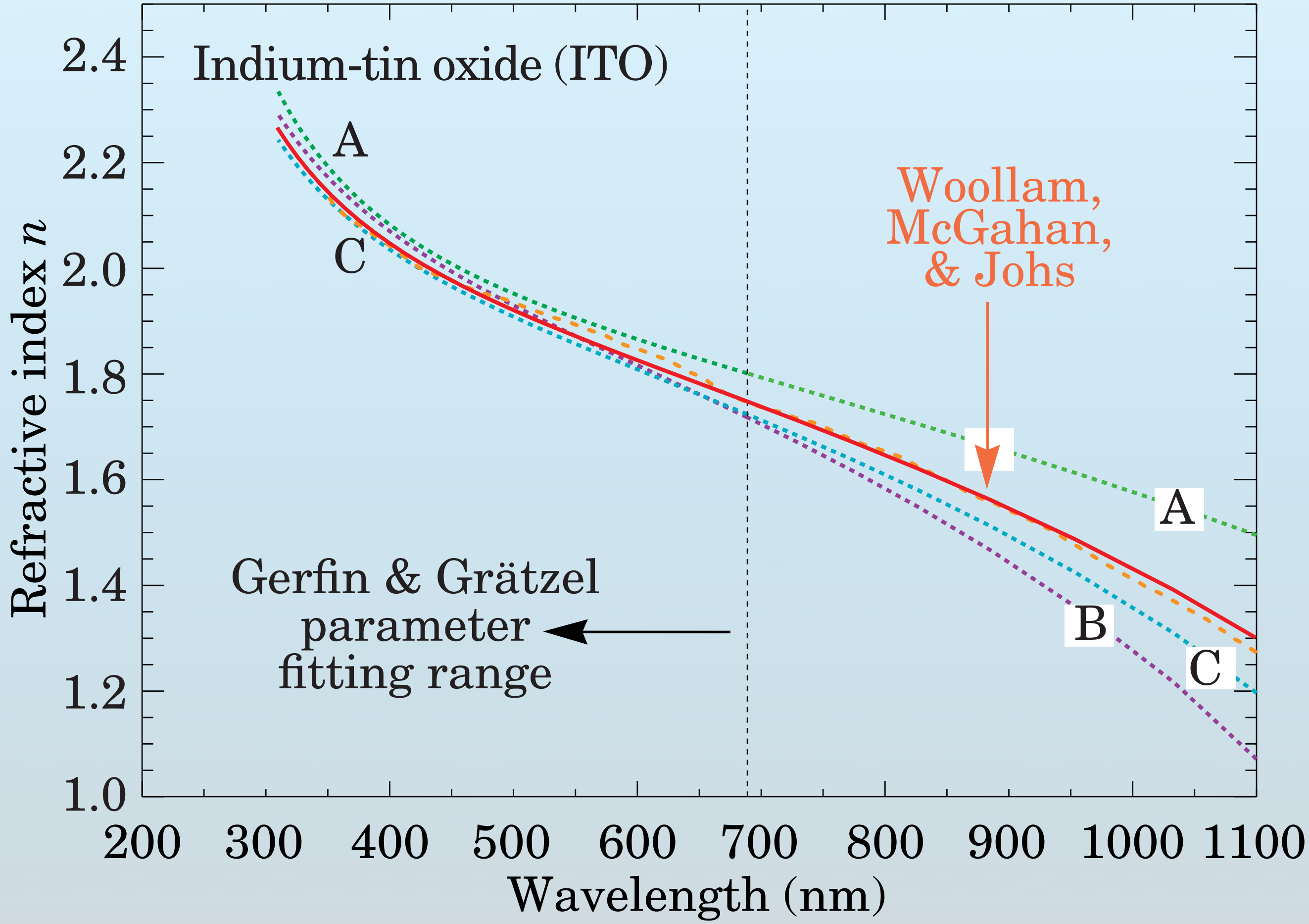
I \propto Re(E*B) \propto Re(nc EE*)
\propto n EE*
Is that the real part of nc or |nc|??
Turns out to be real part.

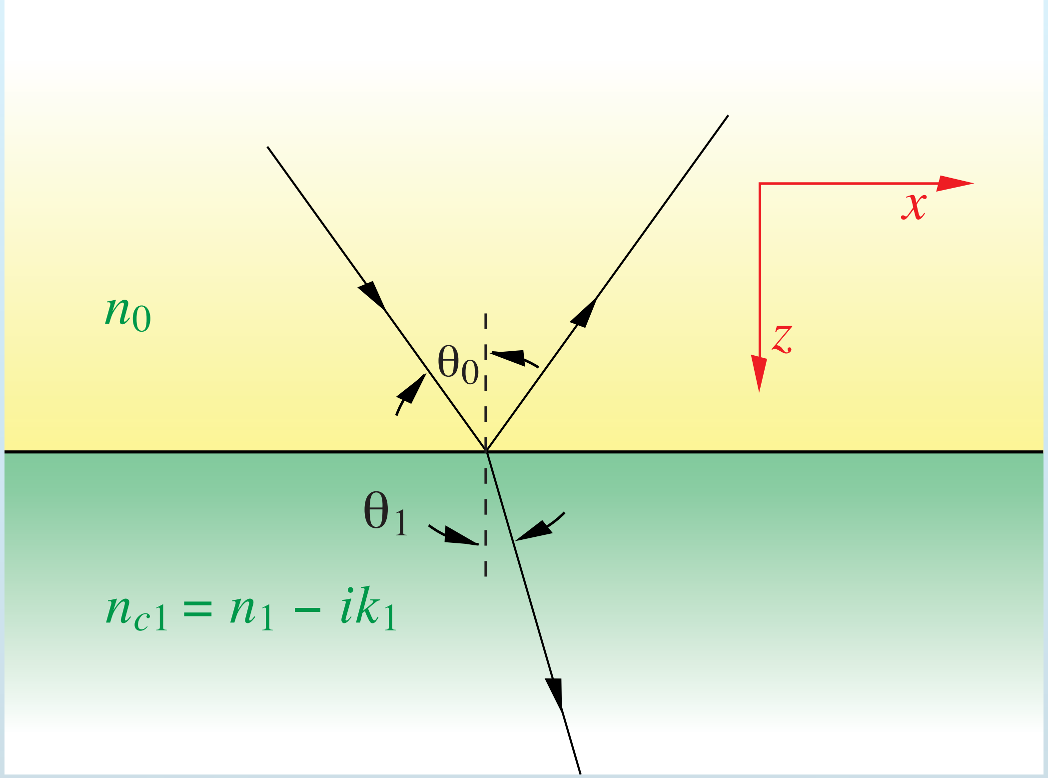
$$I \propto \Re(E^* B) \propto \Re(n_c E E^*) \propto n E E^*$$

Is that $|n_c|$ or $\Re(n_c)$??

$\longrightarrow$ Turns out to be real part.

n_c is the complex index of refraction in a single transit of the *j*th film:


Indium-tin oxide (ITO)
A
C
Woollam, McGahan, & Johs
A
B
C
Gerfin & Grätzel parameter fitting range
Refractive index n
Wavelength (nm)
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
200
300
400
500
600
700
800
900
1000
1100


n_0
θ_0
x
z
θ_1
$n_{c1} = n_1 - ik_1$