Calcback

Nikolai Weidt

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1 What is this?

This is a script to get the complex refractive index $n = n * ik$ from the ellipsometric parameters Δ and Ψ I got from a simulation. The result for

300nm SiO_2 should look like this:

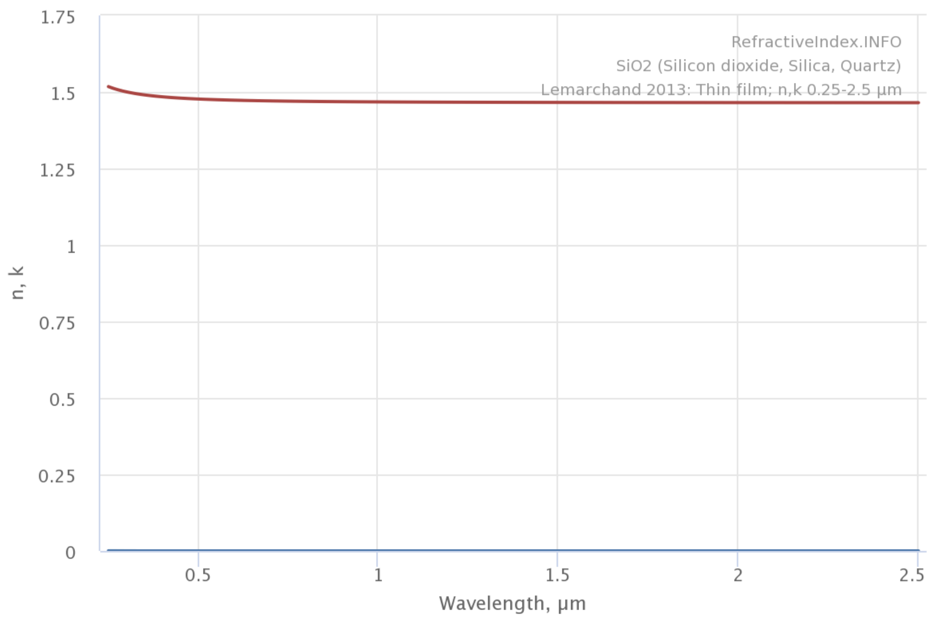


Figure 1: Refractive index should look like this

2 List of Todos:

2.1 TODO Write a loop for all wavelengths after it works for one.

2.2 TODO Then take even more wavelengths (rows)

3 Imports:

```
import numpy as np
import matplotlib
matplotlib.use('Agg')
import matplotlib.pyplot as plt
```

4 Defining some variables:

Defining some variables for later use:

```
CSVFILE = "head300nmSiO2.csv"  # head = only 10 rows of data
phi_i = 70 * np.pi / 180  # converting incident angle from deg (first number) to rad
d_L = 300  # thickness of layer in nm
n_air = 1  # refractive index of air
rerange = 5  # upper limit for real part
imrange = 1  # upper limit for imaginary part
i = 0  # only look at one wavelength (row in csv)
```

5 Read .csv-file:

Read the values into a two dimensional numpy array as [[lambda,Psi,Delta,n_S, k_S],...] (Skip columns 3 and 4)

```
csv = np.loadtxt(CSVFILE, usecols=(0,1,2,5,6),  delimiter=",", skiprows=1)
```

The array looks like this:

```
csv
```

```
[[300.          55.2217535   84.37228319   2.6726       3.0375    ]
 [303.          50.11187439  93.3085011    2.7346       3.0381    ]
 [306.          46.35824553  98.43681392   2.7967       3.0368    ]
 [309.          43.50539341 101.18051798   2.8588       3.0334    ]
 [312.          41.29392865 102.19236832   2.9206       3.0279    ]
 [315.          39.48751217 101.93002      2.9822       3.0205    ]
 [318.          37.90308303 100.64846104   3.0435       3.0109    ]
 [321.          36.47640803  98.54577151   3.1042       2.9994    ]
 [324.          35.12615859  95.72242205   3.1644       2.9858    ]]
```

6 Calculate ρ

6.1 Create a matrix containing every possible refractive index (n+ik):

Change the last number in the "linspaces" to adjust the resolution.

```
lsp_re = np.linspace(1, rerange, 1001)
lsp_im = np.linspace(0.01, imrange, 1001)
re, im = np.meshgrid (lsp_re, lsp_im, copy=False)
n_L = 1j * np.round(im,6) + np.round(re,6)
n_L = n_L.flatten() # create onedimensional array
```

This gives the following matrix:

```
n_L

[1.   +0.01j 1.004+0.01j 1.008+0.01j ... 4.992+1.j   4.996+1.j
 5.   +1.j  ]
```

6.2 Calculate ρ:

6.2.1 First we define some functions:

1. Snell's Law to calculate the refractive angles: Phi is the incident angle for the layer, n1 and n2 are refractive indices of first and second medium. Returns the angle of refraction.

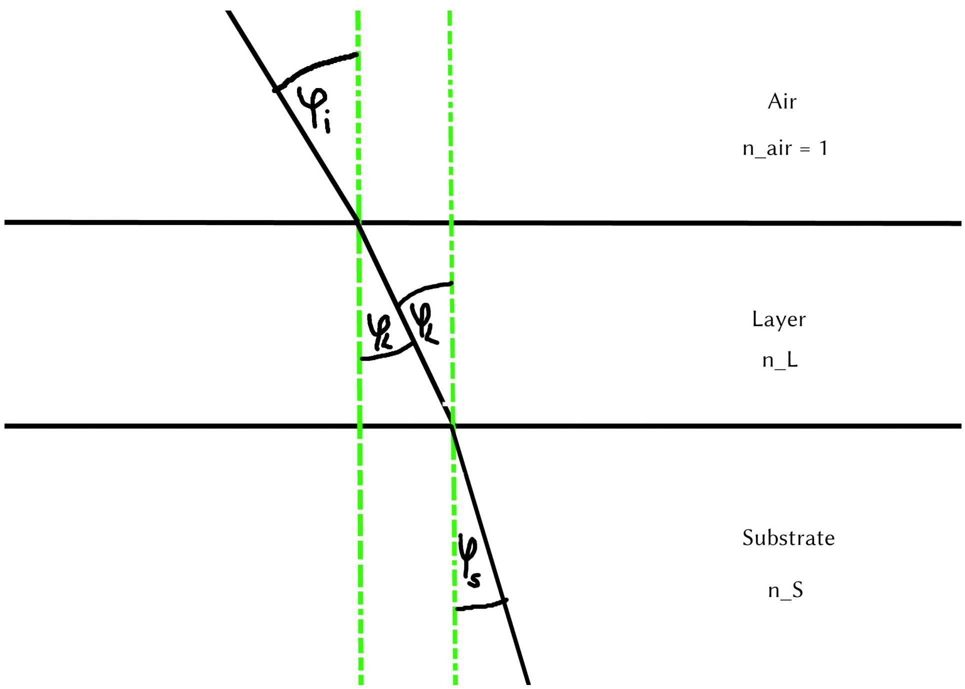


Figure 2: Snell's Law

```
def snell(phi, n1, n2):
    phi_ref = np.arcsin((np.sin(phi) * n1) / n2)
    return phi_ref
```

2. Calculate r_p and r_s with Fresnel equations:

```
def fresnel(n1, phi1, n2, phi2):
    """Takes refractive indices and angles of two layers to calculate the amplituc
    rs = (n1 * np.cos(phi1) - n2 * np.cos(phi2)) / (n1 * np.cos(phi1) + n2 * np.cc
    rp = (n2 * np.cos(phi1) - n1 * np.cos(phi2)) / (n2 * np.cos(phi1) + n1 * np.cc
    return rs, rp
```

3. Calculate ρ for the layer with eq. 5.2 in Spectroscopic Ellipsometry fujiwara2009spectroscopic:

```
def calc_rho(rs_al, rp_al, rs_ls, rp_ls, d_L, n_L, lambda_vac):
    beta = 2 * np.pi * d_L * n_L * np.cos(phi_L) / lambda_vac
    rp_L = (rp_al + rp_ls * np.exp(-2*1j*beta)) / (1 + rp_al * rp_ls * np.exp(-2 *
    rs_L = (rs_al + rs_ls * np.exp(-2*1j*beta)) / (1 + rs_al * rs_ls * np.exp(-2 *
    rho = rp_L / rs_L
    return rho
```

6.2.2 Then we call these functions one after another to calculate ρ:

Get refractive index of the substrate (n_S) and lambda from the csv:

```
lambda_vac = csv[i, 0]
n_S = (csv[i, 3] + 1j * csv[i, 4])
```

Then call the above defined functions

```
phi_L = snell(phi_i, n_air, n_L)
phi_S = snell(phi_L, n_L, n_S)
# Fresnel equations:
# air/layer:
rs_al, rp_al = fresnel(n_air, phi_i, n_L, phi_L)
# layer/substrate:
rs_ls, rp_ls = fresnel(n_L, phi_L, n_S, phi_S)

rho_L = calc_rho(rs_al, rp_al, rs_ls, rp_ls, d_L, n_L, lambda_vac)
```

6.2.3 Identify the best fitting rho with $\rho = \tan(\psi) * e^{i\Delta}$:

```
# psi is in our csv-file at index 1, delta at index 2 at row "i" for lambda
psi = csv[i][1]
delta = csv[i][2]
rho = np.tan(psi) * np.exp(1j * delta)
diff = abs(rho - rho_L)  # magnitude of complex number
idx = np.argmin(diff)  # index of the minimum
minimum = diff[idx]
n = n_L[idx]
print("The layer has the refractive index n_L = ", n)
```

```
The layer has the refractive index n_L =  (4.008+0.15157j)
```

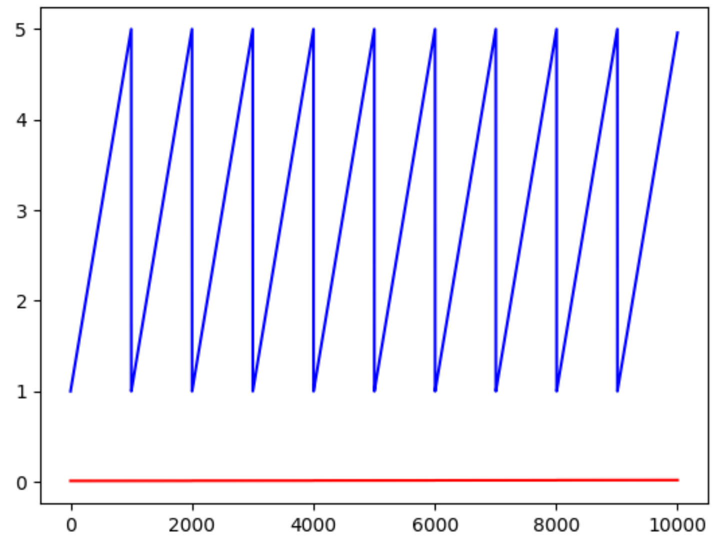
7 Plot some things for checking results:

If we use a high resolution, those plots are not showing much, thats why they are only showing the first 10000 values.

7.1 Plot real and imaginary part of the created n_L matrix:

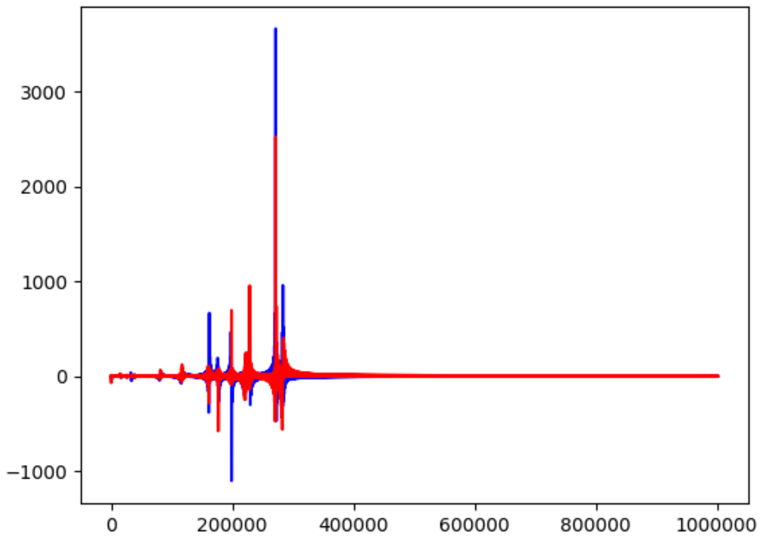
Real part is blue, imaginary is red.

```
fig = plt.figure()
plt.plot(np.real(n_L[:10000]), c='b')
plt.plot(np.imag(n_L[:10000]), c="r")
plt.savefig('n_L.png')
'./n_L.png'
```



7.2 Plot real and imaginary part of $\rho_{\mathbf{L}}$

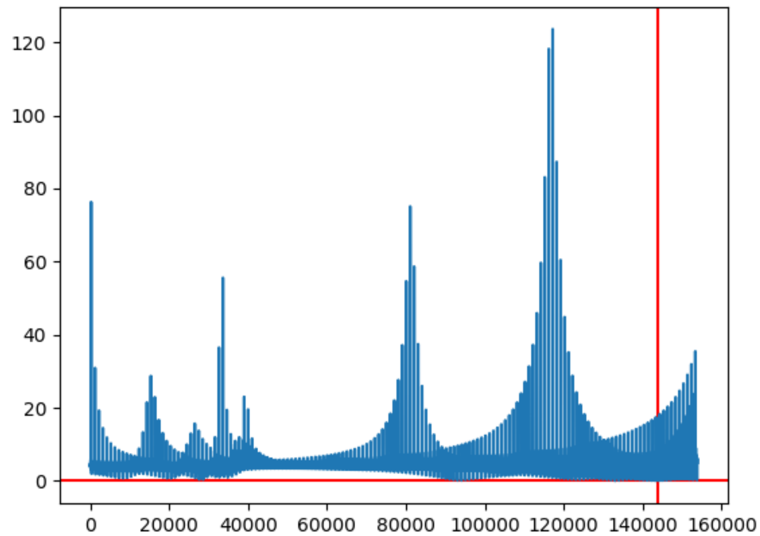
```
fig = plt.figure()
plt.plot(np.real(rho_L), c='b')
plt.plot(np.imag(rho_L), c='r')
plt.savefig('rho_L.png')
"./rho_L.png"
```



7.3 Plot of the difference between ρ_{L} and the given ρ and determined minimum:

The difference is shown in blue, the red lines show the minimum.

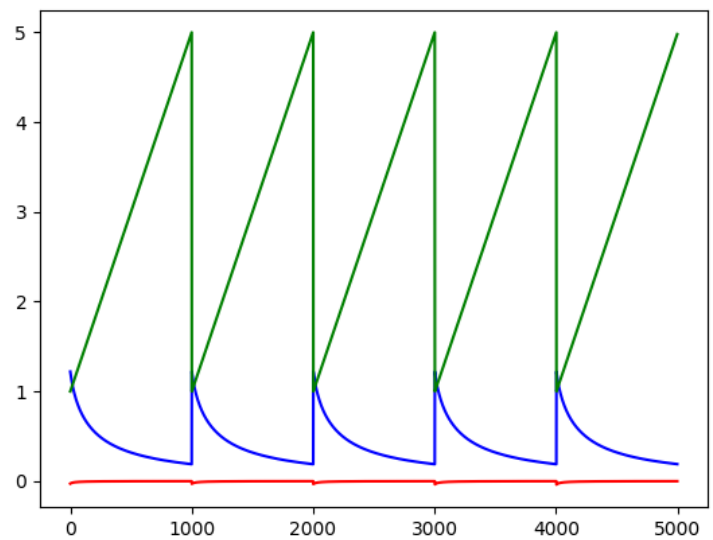
```
fig = plt.figure()
plt.axvline(idx, c='r')
plt.axhline(minimum, c='r')
plt.plot(diff[:idx+10000])
plt.savefig('diff.png')
"./diff.png"
```



7.4 Plot refractive angle $\mathrm{phi_L}$ and $\mathrm{n_L}$:

$\mathrm{n_L}$ is shown in green, real part of $\mathrm{phi_L}$ in blue, imaginary in red. A relation between these should be visible.

```
fig = plt.figure()
plt.plot(np.real(phi_L[:5000]), 'b')
plt.plot(np.imag(phi_L[:5000]), 'r')
plt.plot(np.real(n_L[:5000]), c='g')
plt.savefig('phi_L.png')
"phi_L.png"
```


5
4
3
2
1
0
0
1000
2000
3000
4000
5000