Polman analysis

April 24, 2018

```
In [1]: import os
        import pandas as pd
        import numpy as np
        import matplotlib.pyplot as plt

        %matplotlib notebook
```

1 Equations

Starting equations:

$$T = (1 - R)^2 e^{-\alpha d}$$

as $I_0 = (1 - R)^2$ in Beer-Lambert law. Therefore absorption coefficient α [cm-1]:

$$\alpha = \frac{1}{d} \ln \left(\frac{(1-R)^2}{T} \right)$$

where d is the sample thickness, R and T are reflection and transmission (fractional), respectively. Neglecting fresnel reflection this simplifies to

$$\alpha = -\frac{1}{d} \ln(T).$$

Using the cross-section of OH at 2.73um, $\sigma_{OH} = 1.2E - 19$cm-1, and knowledge that absorption at this wavelength in glass is due to water, we can evaluate the number density of OH [cm-3]

$$N_{OH} = \frac{\alpha}{\sigma_{OH}}$$

[1] DOI: 10.1016/0925-3467(95)00063-1

To convert to ppm: https://doi.org/10.1016/j.vibspec.2008.01.004

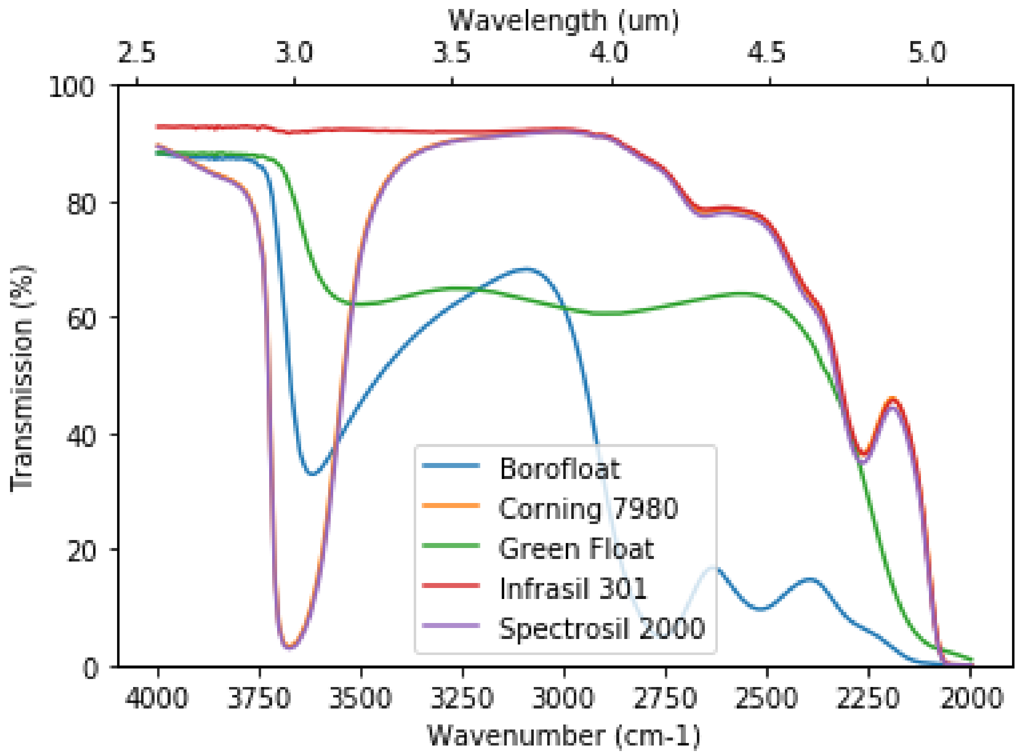
Note: Because the OHabsorption peak shifts slightly depending on the OH concentration, the optimal method is to search for the exact Tmin, instead measuring the Tmin at a fixed wavelength.

```
In [2]: # Thickness of samples (cm)
        d = 0.11

        # Absorption cross section of OH in glass (cm2) @ 2.73um or 3662cm-1
        sig_OH = 1.2E-19
```

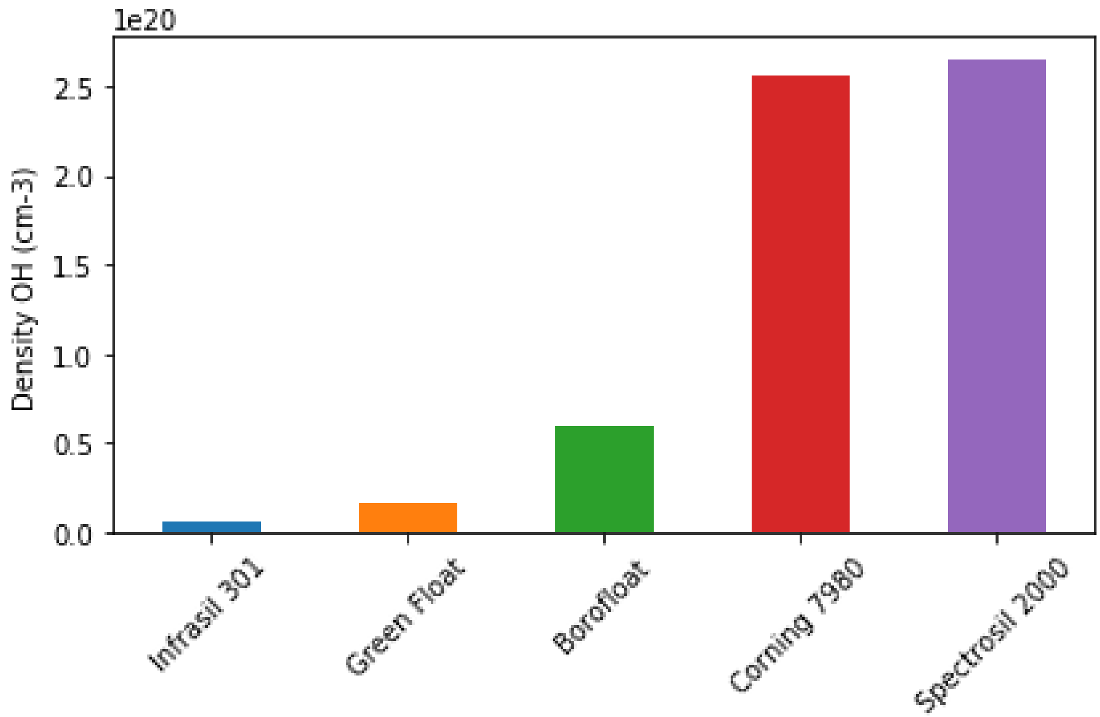
2 FTIR

In [3]:
```
path = './FTIR/'
files = [x for x in os.listdir(path) if '.DPT'in x]

fig, ax1 = plt.subplots()
ax2 = ax1.twiny()

store = {}
for f in files:
    result = np.genfromtxt(path + f)
    f = f.split('.')[0]
    # Wavenumber
    x = result[:, 0]
    # Transmission
    y = result[:, 1]
    ax1.plot(x, 100*y, label=f)

    # Store number of OH
    y = y[np.where(x >= 3663)[0][0]]
    alpha = -np.log(y)/d
    store[f] = alpha / sig_OH

# In wavenumber so x is descending
ax1.set_xlim(ax1.get_xlim()[::-1])
ax1.set_xlabel('Wavenumber (cm-1)')
ax1.set_ylabel('Transmission (%)')
ax1.legend()
ax2.set_ylim(0, 100)
lb, ub = ax1.get_xlim()
ax2.set_xlim(10000/lb, 10000/ub)
ax2.set_xlabel('Wavelength (um)')
```

Out[3]:
```
Text(0.5,0,'Wavelength (um)')
```




```
In [4]: store = pd.Series(store, name='Sample')
        store = store.sort_values()

        fig, ax = plt.subplots()
        store.plot(kind='bar', rot=45)
        ax.set_ylabel('Density OH (cm-3)')
        plt.tight_layout()
```

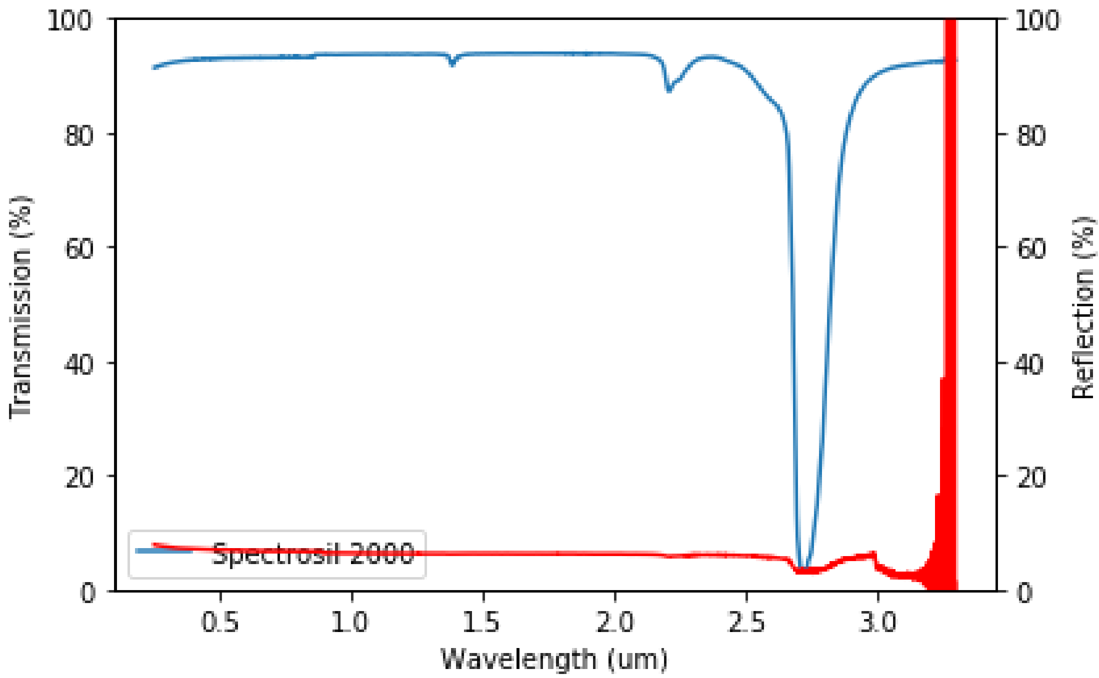


3 Individual Sample

In [5]:
```
fig, ax1 = plt.subplots()
ax2 = ax1.twinx()

path = './UVVIS/Transmission/data/'
f = [x for x in os.listdir(path) if '.csv'in x and 'Spectrosil' in x][0]
result = np.genfromtxt(path + f, delimiter=',', skip_header=1)
f = f.split('.')[0]
# Wavelength (um)
x = result[:, 0] / 1000
# Transmission
y = result[:, 1] / 100
ax1.plot(x, 100*y, label=f)
ax1.legend()
ax1.set_xlabel('Wavelength (um)')
ax1.set_ylabel('Transmission (%)')
ax1.set_ylim(0, 100)

path = './UVVIS/URA/'
f = [x for x in os.listdir(path) if '.csv'in x and 'Spectrosil' in x][0]
result = np.genfromtxt(path + f, delimiter=',', skip_header=1)
f = f.split('.')[0]
```

```
    # Wavelength (um)
    x = result[:, 0] / 1000
    # Reflection
    y = result[:, 1] / 100

    ax2.plot(x, 100*y, label=f, color='red')
    ax2.set_ylabel('Reflection (%)')
    ax2.set_ylim(0, 100)
```

```
Out[5]: (0, 100)
```

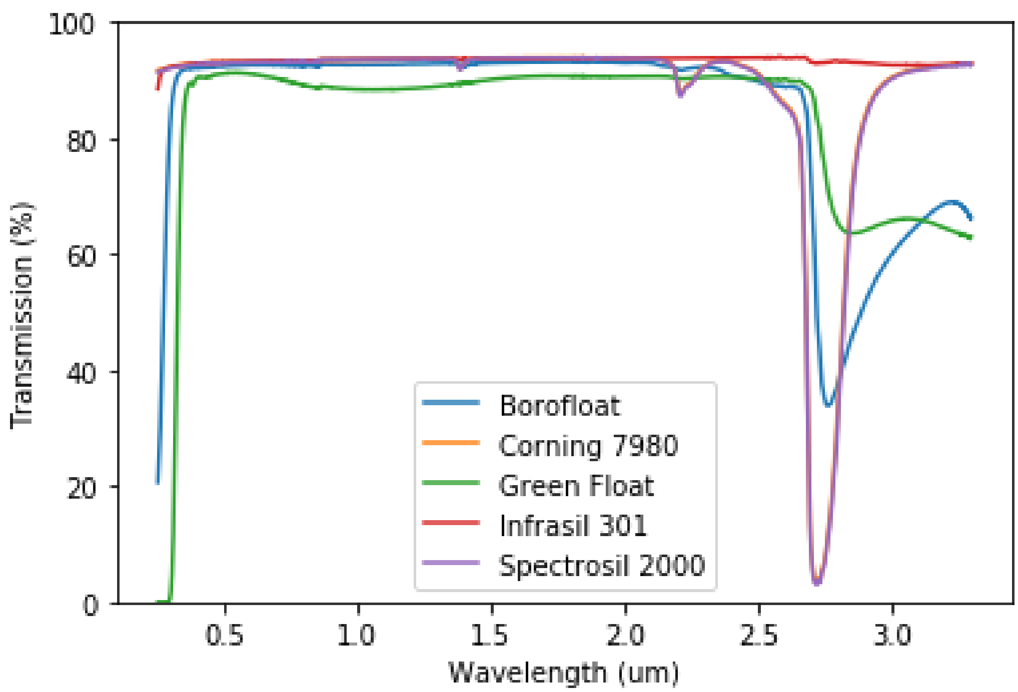


4 UV-VIS

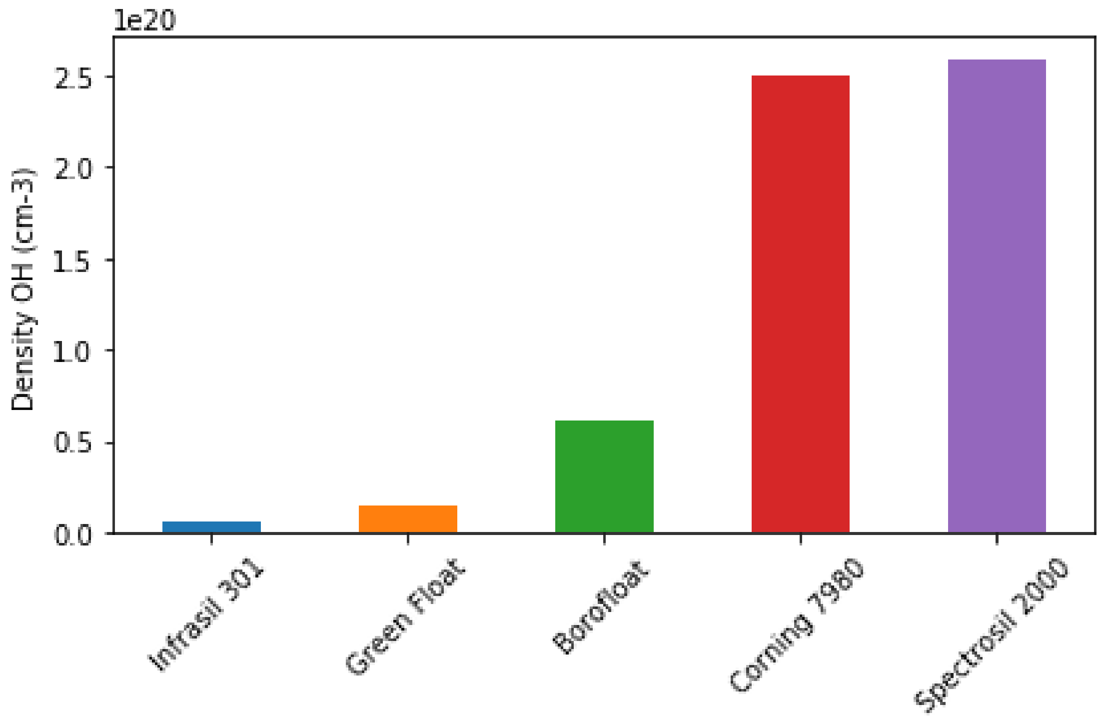
```
In [14]: path = './UVVIS/Transmission/data/'
         files = [x for x in os.listdir(path) if '.csv'in x and 'Correction' not in x]

         fig, ax1 = plt.subplots()
         store = {}
         for f in files:
             result = np.genfromtxt(path + f, delimiter=',', skip_header=1)
             f = f.split('.')[0]
             # Wavelength (um)
             x = result[:, 0] / 1000
             # Transmission
```

```
        y = result[:, 1] / 100

        ax1.plot(x, 100*y, label=f)

        # Store number of OH
        y = y[np.where(x == 2.73)[0][0]]
        alpha = np.log(y)/-d
        store[f] = alpha / sig_OH

    ax1.legend()
    ax1.set_xlabel('Wavelength (um)')
    ax1.set_ylabel('Transmission (%)')
    ax1.set_ylim(0, 100)
```

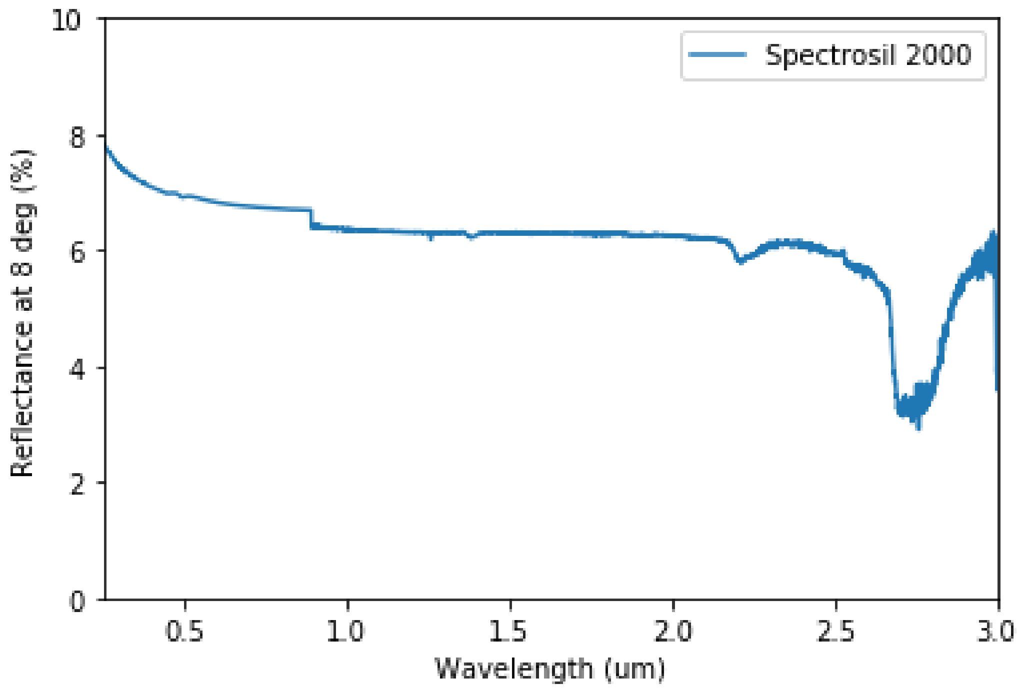
Out[14]: (0, 100)




```
In [15]: store = pd.Series(store, name='Sample')
         store = store.sort_values()

         fig, ax = plt.subplots()
         store.plot(kind='bar', rot=45)
         ax.set_ylabel('Density OH (cm-3)')
         plt.tight_layout()
```




```
In [16]: path = './UVVIS/URA/'
         files = [x for x in os.listdir(path) if '.csv'in x and 'Correction' not in x]

         fig, ax1 = plt.subplots()
         store = {}
         for f in files:
             result = np.genfromtxt(path + f, delimiter=',', skip_header=1)
             f = f.split('.')[0]
             # Wavelength (um)
             x = result[:, 0] / 1000
             # Transmission
             y = result[:, 1] / 100

             ax1.plot(x, 100*y, label=f)

         ax1.legend()
         ax1.set_xlabel('Wavelength (um)')
         ax1.set_ylabel('Reflectance at 8 deg (%)')
         ax1.set_ylim(0, 10)
         ax1.set_xlim(.25, 3)

Out[16]: (0.25, 3)
```



5 Plot UV-VIS and FTIR data together

```
In [20]: fig, ax1 = plt.subplots()

         path = './UVVIS/Transmission/data/'
         files = [x for x in os.listdir(path) if '.csv'in x and 'Correction' not in x]

         # Color map - unique for each sample
         samples = [f.split('.')[0] for f in files]
         colors = np.arange(len(samples))
         color_dict = dict(zip(samples, colors))
         import matplotlib.colors as mcolors
         import matplotlib.cm as cmx
         cNorm  = mcolors.Normalize(vmin=0, vmax=len(samples)-1)
         scalarMap = cmx.ScalarMappable(norm=cNorm, cmap=plt.get_cmap('tab10') )

         for f in files:
             result = np.genfromtxt(path + f, delimiter=',', skip_header=1)
             f = f.split('.')[0]
             # Wavelength (um)
             x = result[:, 0] / 1000
             # Transmission
             y = result[:, 1] / 100
```

```
    colorVal = scalarMap.to_rgba(color_dict[f])
    ax1.plot(x, 100*y, color=colorVal)

path = './FTIR/'
files = [x for x in os.listdir(path) if '.DPT'in x]
for f in files:
    result = np.genfromtxt(path + f)
    f = f.split('.')[0]
    # Wavenumber
    x = 10E3/result[:, 0]
    # Transmission
    y = result[:, 1]
    # NOTE 1% OFFSET BETWEEN UVVIS AND FTIR. NOT SURE WHICH IS RIGHT.
#     y += 0.01

    colorVal = scalarMap.to_rgba(color_dict[f])
    ax1.plot(x, 100*y, label=f, color=colorVal)

ax1.legend()
ax1.set_xlabel('Wavelength (um)')
ax1.set_ylabel('Transmission (%)')
ax1.set_ylim(0, 100)
# ax1.set_xlim(0.25, 5)
```

Out[20]: (0, 100)