

Exercise 2.1 Solution

A) The material absorbs the light through:

$$I(l) = I_0 e^{-\alpha l}$$

Where $I(l)$ is the intensity of light through a layer of matter with thickness l , I_0 is the initial intensity, α is the absorption coefficient. Do not confuse the dimensional absorption coefficient $[\alpha] = m^{-1}$ and the dimensionless one k :

$$\alpha = \frac{4\pi k}{\lambda}$$

For the absorption to be 90%, we need to have the thickness of the material $l_{90\%}$:

$$\begin{aligned} \frac{I(l_{90\%})}{I_0} &= 0.1 \\ e^{-\alpha l_{90\%}} &= 0.1 \\ l_{90\%} &= -\frac{\ln 0.1}{\alpha} = -\frac{\lambda \ln 0.1}{4\pi k} \end{aligned}$$

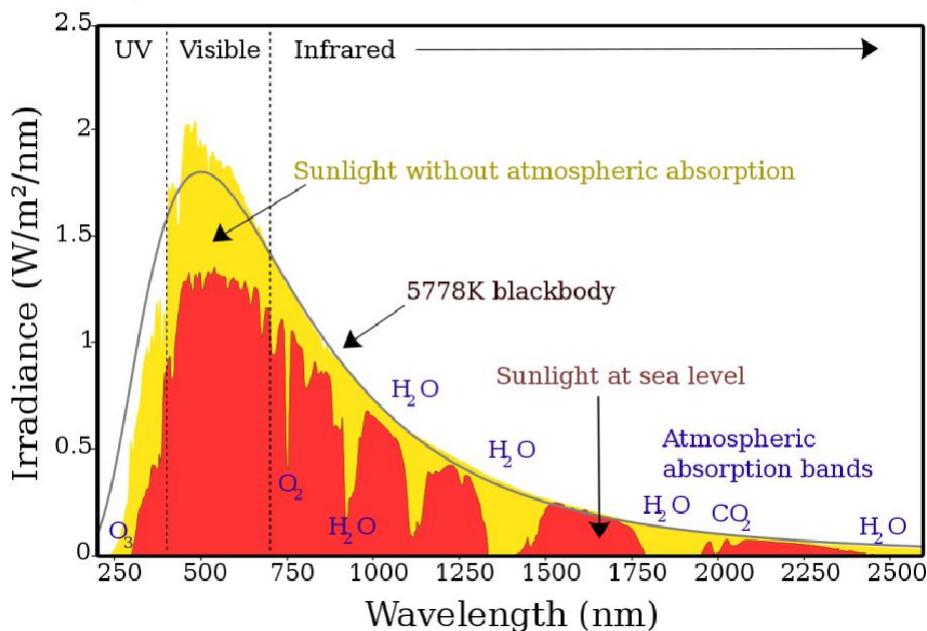
B) For $\lambda = 700 nm$:

$\lambda = 700 nm$	n	k	α	$\frac{1}{\alpha}$	$l_{90\%}$	R
Glass	1.52	$15 \cdot 10^{-7}$	$2.69 \cdot 10^{-1} \text{ cm}^{-1}$	3.7 cm	8.6 cm	0.0426
Silicon	4	0.011	$1.97 \cdot 10^3 \text{ cm}^{-1}$	$5.2 \cdot 10^{-4} \text{ cm}$	$1.2 \cdot 10^{-3} \text{ cm}$	0.360
Heptametine cyanine	1	0.9	$1.62 \cdot 10^5 \text{ cm}^{-1}$	$6.2 \cdot 10^{-6} \text{ cm}$	$1.4 \cdot 10^{-5} \text{ cm}$	0.168
SnO_2	1.95	0.06	$1.08 \cdot 10^4 \text{ cm}^{-1}$	$9.3 \cdot 10^{-5} \text{ cm}$	$2.1 \cdot 10^{-4} \text{ cm}$	0.104
$\text{CH}_3\text{NH}_3\text{PbI}_3$	2.5	0.2	$3.59 \cdot 10^4 \text{ cm}^{-1}$	$2.8 \cdot 10^{-5} \text{ cm}$	$6.4 \cdot 10^{-5} \text{ cm}$	0.186

C) Some notes about considered materials:

Photovoltaics (PV) is the conversion of light into electricity using semiconducting materials that exhibit the photovoltaic effect. For electricity generation application, and for solar cells in particular, firstly the material should absorb the light emitted by the sun. The sun emission spectrum is shown below. As we can see, sun emission is concentrated mostly in visible and near IR ranges. Thus, the prerequisites for solar cell materials is that absorbs strongly in the visible and NIR region. The other requirement is that the material is a semiconductor. However, if we just focus on the optical properties (absorption and reflection) we can already draw some conclusions.

Spectrum of Solar Radiation (Earth)



If the absorption of material is low, we need to use a thick layer to absorb. As you can see from the table, the glass is almost transparent in the visible range, so we need a thick layer of glass (almost 10 cm) to absorb 90% of incoming intensity. If we compare silicon and SnO_2 , we see that the absorption is twice for SnO_2 then the value for silicon. So, we need six times thicker silicon to absorb the same intensity.

The second thing that should be taken into account is reflectance. We see, that for some materials like silicon the reflective loss is quite high (about 36%), so it is important to use antireflective coating to increase the amount of light that penetrates inside the material.

Organic materials, for example, heptamethine cyanine has strong absorption only in 600-900 nm, $k = 0$ beyond this region. Therefore, the material is transparent for other wavelengths including visible range 300-600 nm, making it useful for transparent solar cells.

Lead-halide perovskite semiconductors are very attractive for their suitable optical properties and the processing possibilities from solution. They may become one of the important photovoltaic materials in future solar cell technology.

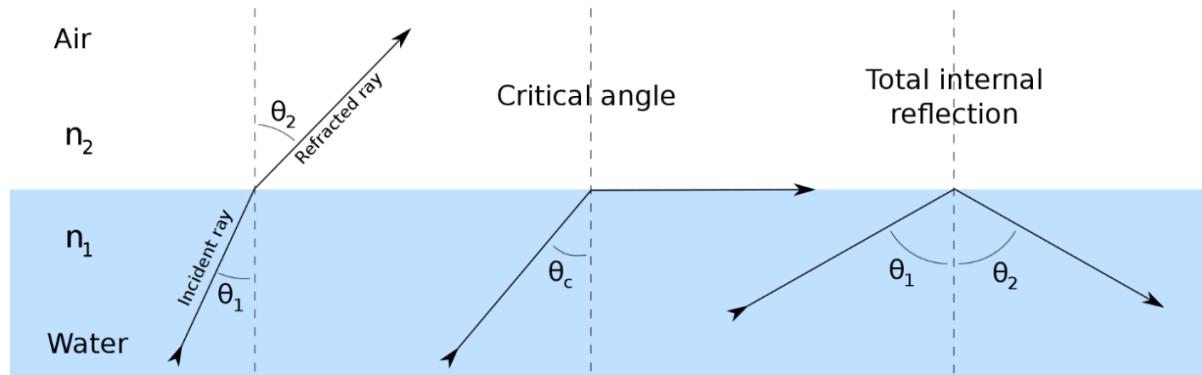
Exercise 2.2 Solution

A) ATR stands for Attenuated Total Reflectance. It is most widely used sampling methodology for FTIR spectroscopy. The sample (solid or liquid) is placed onto the ATR crystal. Solid samples are usually pressed to ensure optimal contact between the sample and the crystal. The light (usually infrared) travels through a crystal at least once at the crystal-sample interface. During the internal reflection, a part of the IR light penetrates into the sample, where it can be absorbed. Penetration depth of the evanescent wave into the sample is defined by the refractive index difference between the sample and the ATR crystal. The order of magnitude of penetration depth is usually about hundredth of nanometers- tens of microns.

To increase the sensitivity, multiple reflections undergoing total internal reflection can be used inside the crystal. In this case the light penetrates inside the material studied by ATR several times, effectively increasing the signal.

A way to increase sensitivity involves increase in the contact area of the material with the surface of diamond by utilization of liquid samples.

Angle dependence of penetration depth (see part C) allows to increase or decrease this value. For some specific cases of particular compounds, diamond surface functionalized by deposition of thin films, that would bind the compound of interest.



As the result of the lecture, we know that, if the angle is greater than the critical angle, the light totally reflects from the interface. This phenomenon is called total internal reflection.

For water-air interface the critical angle is:

$$\theta_c^{\text{water-air}} = \sin^{-1} \frac{1}{1.33} \approx 48.8^\circ$$

For diamond-air interface:

$$\theta_c^{\text{diamond-air}} = \sin^{-1} \frac{1}{2.417} \approx 24.44^\circ$$

Note, that despite there is no explicit dependence on wavelength in the critical angle, in fact the refractive index depends on wavelength, so the critical angle depends on wavelength as well:

$$\theta_c(\omega) = \sin^{-1} \frac{n_2(\omega)}{n_1(\omega)}$$

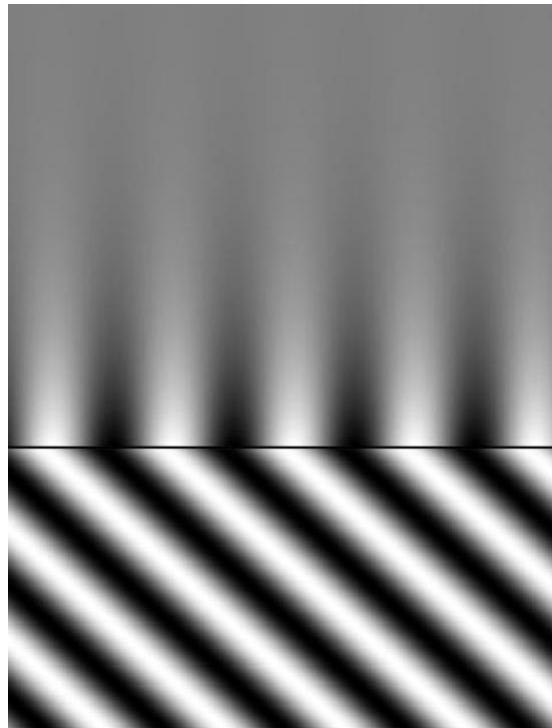
For $\theta_c^{\text{diamond-air}}$ calculation we used the averaged refractive index of diamond for visible range. However, we can compare how it changes if we use the refractive index for MIR range. According to [1], the refractive index of diamond for 1500 cm⁻¹ (6666 nm) is 2.376, that results in difference about 2%.

C) From the lecture we know that penetration depth could be expressed as:

$$d = \frac{1}{\kappa} = 1/\kappa_0 \sqrt{n_I^2 \sin^2 \theta_I - n_T^2}$$

Where, $\kappa_0 = \frac{\lambda_0}{2\pi}$, $\theta_I = \pi/4$

Answer: $d \approx 766 \text{ nm}$

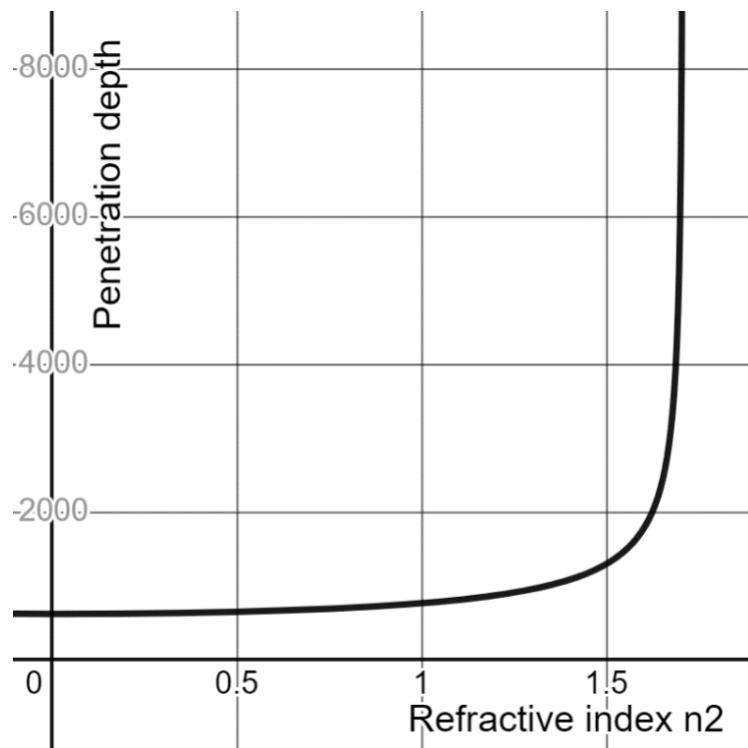


Depiction of an incident sinusoidal plane wave (bottom) and the associated evanescent wave (top)

D) In case of liquid, we should compare the refractive index of liquid and the refractive index of diamond. The behavior of the penetration depth is shown below.

It is clear, that when the refractive index of the liquid reaches the effective refractive index of the diamond, the penetration depth becomes infinite since it is not the case of total internal reflection anymore. The critical angle of total internal reflection becomes greater than the incident angle and the wave refracts to the liquid without creating the evanescent wave with decaying amplitude.

To learn more about the nature of the evanescent wave you can check the article [2].



References:

- [1] Edwards, D. F., & Ochoa, E. (1981). Infrared refractive index of diamond. *JOSA*, 71(5), 607-608.
- [2] Milosevic, M. (2013). On the nature of the evanescent wave. *Applied spectroscopy*, 67(2), 126-131.