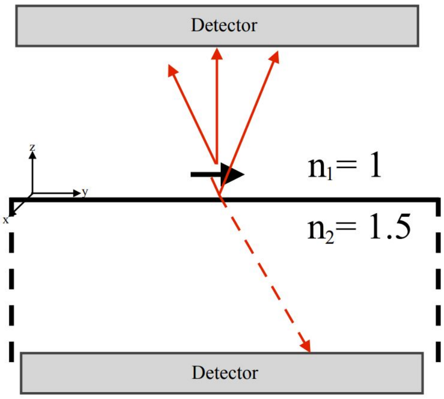
1 A Dipole on an Air/Dielectric Interface

- For a dipole sitting on an air/dielectric interface ($n_1 = 1, n_2 = 1.5$) calculate the ratio between the energy radiated into the upper half-space and the energy radiated into the lower half-space.
- Perform the calculations separately for a horizontal and a vertical dipole.
- Additionally, please calculate the apparent quantum yield, which is defined as the ratio between the power radiated in the lower half space and the total dissipated power.

We consider a dipole on a surface of transparent material (e.g. glass) and calculate the detected light on top and under the surface.



$$\mathbf{E}(r) = \omega^2 \mu_0 \mu_1 \overleftrightarrow{G}(r_0, r)\mu$$

where μ is the electric dipole. This equation indicates that we only need to find the dyadic Green function in the problem situation. In general this Green function is

$$\overleftrightarrow{G} = \frac{i}{8\pi^2} \iint_{-\infty}^{\infty} \overleftrightarrow{M} e^{i[k_x(x-x_0)+k_y(y-y_0)+k_{z_1}|z-z_0|]} \mathrm{d}k_x \, \mathrm{d}k_y$$

For upper part the detector can collect the emitted and reflected light. In order to calculate the reflected and emitted light we have to find the Green function in each case. We already calculated emitted light from a dipole for free space. In Free space $\overleftrightarrow{M}$ is:

$$\overleftrightarrow{M} = \frac{1}{k_1^2 k_{z_1}} \begin{pmatrix} k_1^2 - k_x^2 & -k_x k_y & \pm k_x k_{z_1} \\ -k_x k_y & k_1^2 - k_y^2 & \pm k_y k_{z_1} \\ \pm k_x k_{z_1} & \pm k_y k_{z_1} & k_1^2 - k_{z_1}^2 \end{pmatrix}$$

The value $r_0(x_0, y_0, z_0) = 0$ is the position of the dipole. If $z = 0$ is the position of interface then the negative sign is for $z > z_0$ and the positive sign is for $z < z_0$. Here, the value:

$$k_{z_1} = \sqrt{k_1^2 - (k_x^2 + k_y^2)}$$
$$k_1 = \frac{\omega}{c}\sqrt{\epsilon_1\mu_1}$$
$$\sqrt{k_x^2 + k_y^2} = k_1 \sin\theta$$

In order to use Fresnel reflection equation we should split $\overleftrightarrow{G}$ to s and p polarization and as a result decompose $\overleftrightarrow{M}$.

$$\overleftrightarrow{M}(k_x, k_y) = \overleftrightarrow{M}^s(k_x, k_y) + \overleftrightarrow{M}^p(k_x, k_y)$$

$$\overleftrightarrow{M}^p = \frac{1}{k_1(k_x^2 + k_y^2)} \begin{pmatrix} k_x^2 k_{z_1} & k_x k_y k_{z-1} & \pm k_x(k_x^2 + k_y^2) \\ k_x k_y k_{z_1} & k_y^2 k_{z_1} & \pm k_y(k_x^2 + k_y^2) \\ \pm k_x(k_x^2 + k_y^2) & \pm k_y(k_x^2 + k_y^2) & (k_x^2 + k_y^2)^2/k_{z_1} \end{pmatrix}$$
$$\overleftrightarrow{M}^s = \frac{1}{k_{z_1}(k_x^2 + k_y^2)} \begin{pmatrix} k_y^2 & -k_x k_y & 0 \\ -k_x k_y & k_x^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

To calculate the dipole reflected field we simply multiply the individual plane waves in $\overleftrightarrow{G}$ with the corresponding Fresnel reflection coefficient r^s and r^p.

$$r^p(k_x, k_y) = \frac{\epsilon_2 k_{z_1} - \epsilon_1 k_{z_2}}{\epsilon_2 k_{z_1} + \epsilon_1 k_{z_2}}$$
$$r^s(k_x, k_y) = \frac{\mu_2 k_{z_1} - \mu_1 k_{z_2}}{\mu_2 k_{z_1} + \mu_1 k_{z_2}}$$

$$\overleftrightarrow{M^s}_{ref} = r^s(k_x, k_y) \cdot \overleftrightarrow{M}^s$$
$$\overleftrightarrow{M^p}_{ref} = r^p(k_x, k_y) \cdot \overleftrightarrow{M}^p$$

$$\overleftrightarrow{G}_{ref}(r, r_0) = \frac{i}{8\pi^2} \iint\limits_{-\infty}^{\infty} [\overleftrightarrow{M^s}_{ref} + \overleftrightarrow{M^p}_{ref}] e^{i[k_x(x-x_0) + k_y(y-y_0) + k_{z_1}(z+z_0)]} \mathrm{d}k_x \, \mathrm{d}k_y$$

The electric field of upper half-space is

$$\mathbf{E}(r) = \omega^2 \mu_0 \mu_1 [\overleftrightarrow{G}_0 + \overleftrightarrow{G}_{ref}]\mu$$

For transmitted part we have the same scenario

$$t^s(k_x, k_y) = \frac{2\mu_2 k_{z_1}}{\mu_2 k_{z_1} + \mu_1 k_{z_2}}$$
$$t^p(k_x, k_y) = \frac{2\epsilon_2 k_{z_1}}{\epsilon_2 k_{z_1} + \epsilon_1 k_{z_2}} \sqrt{\frac{\mu_2 \epsilon_1}{\mu_1 \epsilon_2}}$$

$$\overleftrightarrow{M^s}_{tr} = t^s(k_x, k_y) \cdot \overleftrightarrow{M^s}$$
$$\overleftrightarrow{M^p}_{tr} = t^p(k_x, k_y) \cdot \overleftrightarrow{M^p}$$

$$\overleftrightarrow{G}_{tr}(r, r_0) = \frac{i}{8\pi^2} \iint\limits_{-\infty}^{\infty} [\overleftrightarrow{M^s}_{tr} + \overleftrightarrow{M^p}_{tr}] e^{i[k_x(x-x_0)+k_y(y-y_0)+k_{z_2}z+k_{z_1}z_0]} \mathrm{d}k_x \, \mathrm{d}k_y.$$

The electric field of lower half-space is

$$\mathbf{E}(r) = \omega^2 \mu_0 \mu_1 \overleftrightarrow{G}_{tr} \mu$$

We should put each Green function in magnetic field equation.

$$\mathbf{H}(r) = -i\omega[\nabla \times \overleftrightarrow{G}(r_0, r)]\mu$$

and then using the Poynting vector to find power density.

$$\langle \mathbf{S} \rangle = \frac{1}{2} \mathrm{Re}\{\mathbf{E} \times \mathbf{H}^*\}$$

For the calculatiion of $P_\uparrow$ and $P_\downarrow$, we mucst calculate the far-field pattern.

The radiation pattern can be written as:

$$P_i(\Omega)\mathrm{d}\Omega = r^2 \ < \vec{S_j} > \cdot \hat{n_\Omega}$$

So, for $P_\uparrow$:

$$\frac{P_\uparrow(\Omega)}{P_0} = \frac{3}{8\pi}\frac{1}{P^2}\Big[P_z^2 \sin^2\theta |\phi^1|^2 + \cos^2\theta \ |\phi^1|^2 [P_x \ \cos\phi + P_y \ \sin\phi]^2 + [P_x \ \sin\phi - P_y \ \cos\phi]^2 \ |\phi_1^{(3)}|^2 + P_z\Big[[P_x \ \cos\phi + P_y \ \sin\phi]\cos\theta \ \ \sin\theta \ [\phi_1^{(1)} + \phi_1^*(2) + ...c.c.\Big]\Big]$$

Similarly for $P_\downarrow$

$$\frac{P_\uparrow(\Omega)}{P_0} = \frac{3}{8\pi}\frac{1}{P^2}\Big[P_z^2 \sin^2\theta |\phi^1|^2 + \cos^2\theta \ |\phi^1|^2 [P_x \ \cos\phi + P_y \ \sin\phi]^2 + [P_x \ \sin\phi - P_y \ \cos\phi]^2 \ |\phi_2^{(3)}|^2 + P_z\Big[[P_x \ \cos\phi + P_y \ \sin\phi]\cos\theta \ \ \sin\theta \ [\phi_2^{(1)} + \phi_2^*(2) + ...c.c.\Big]\Big]$$

Considering $z_0 = 0$ and $\rho = 0$ we can write:

$$\phi_1^{(1)} = 1 + r^p(\theta)$$

$$\phi_1^{(2)} = 1 - r^p(\theta)$$

$$\phi_1^{(3)} = 1 + r^s(\theta)$$

$$\phi_3^{(1)} = \frac{n_2}{n_1} \frac{t^p \cos\theta}{\sqrt{\frac{n_1^2}{n_2^2} - \sin^2\theta}}$$

$$\phi_3^{(2)} = -\frac{n_2}{n_1} \times t^p$$

$$\phi_3^{(3)} = \frac{\cos\theta}{\sqrt{\frac{n_1^2}{n_2^2} - \sin^2\theta}} \times t^s$$

$$\tilde{S} = \sqrt{\frac{n_1^2}{n_2^2} - \sin^2\theta}$$

Power in the upper space:

$$P_\uparrow = \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi/2} \sin\theta d\theta \times P_\uparrow(\Omega)$$

$$\int_0^{2\pi} \cos^2\phi \mathrm{d}\phi = \int_0^{2\pi} \sin^2\phi \mathrm{d}\phi = \pi$$

$$P_\uparrow = \frac{3\pi}{8\pi} \frac{P_0}{P^2} \int_0^{\pi/2} \Bigg[2\ P_z^2\ \sin^2\theta\ |1 + r^p(\theta)|^2 + \cos^2\theta\ \ [P_x^2 + P_y^2]\ |1 - r^p(\theta)|^2 + [P_x^2 + P_y^2]\ |1 + r^s(\theta)|^2 \Bigg] \sin\theta\ \mathrm{d}\theta$$

$$P_\downarrow = \frac{3\pi}{8\pi} \int_{\pi/2}^{\pi} \frac{P_0}{P^2} \Bigg[2\ P_z^2\ \sin^2\theta\ [\frac{n_1}{n_2}]^2\ +\ \frac{|t^p|^2\cos^2\theta}{\frac{n_1^2}{n_2^2} - \sin^2\theta} + [P_x^2 + P_y^2]\ \cos^2\theta\ [\frac{n_1}{n_2}]^2\ |t^p|^2\ +\ [P_x^2 + P_y^2] \frac{|t^s|^2\cos^2\theta}{\frac{n_1^2}{n_2^2} - \sin^2\theta} \Bigg]\ \sin\theta\ \mathrm{d}\theta$$

Consider $z_0 = 0$, we can write $P_\uparrow^{||}$ as follows:

$$P_\uparrow^{||} = P_0 \left[\frac{1}{2} + \frac{3}{8} \int_0^1 \left[sS_z \, |r^p|^2 + \frac{s}{S_z} \, |r^s|^2 \right] ds - \frac{3}{4} \int_0^1 \mathrm{Re}\Big\{ \, sS_z \, r^p - \frac{s}{S_z} r^s \Big\} \mathrm{d}s \right]$$

we can write $P_\uparrow^{\perp}$ as follows:

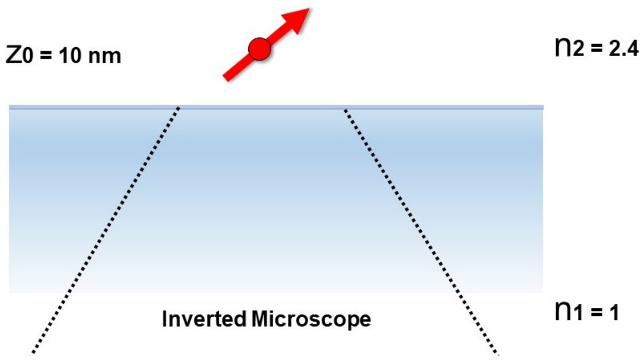
$$P_\uparrow^{\perp} = P_0 \left[\frac{1}{2} + \frac{3}{4} \int_0^1 \left[\frac{s^3}{S_z} \, |r^p|^2 \right] ds + \frac{3}{2} \int_0^1 \mathrm{Re}\Big\{ \, \frac{s^3}{S_z} r^p \Big\} \mathrm{d}s \right]$$

For $P_\downarrow$:

$$P_\downarrow = P_\downarrow(allowed) + P_\downarrow(forbidden)$$

2 Outcoupling Efficiency of a Dipole out of a Diamond Matrix

- Consider a dipole (SiV color center, $\lambda = 738$ nm) located 10 nm inside a semi-infinte diamond medium ($n = 2.4$). Calculate the apparent quantum yield of the dipole for vertical and horizontal orientation with respect to the interface with air using geometrical-optics arguments. Consider light collection in the air medium ($n = 1$).



To do this correctly, take $z_o = 10$ nm and the previous expressions for $P_\uparrow$ and $P_\downarrow$.
We know the expression for the critical angle:

$$\theta_c = \arcsin\left(\frac{n_1}{n_2}\right) \simeq \arcsin\left(\frac{1}{2.4}\right)$$

$$\arcsin\left(\frac{1}{2.4}\right) \simeq \arcsin(0.24)$$

$$\theta_c \simeq 24.6^\circ$$

Thus, we have to consider the emission of the dipole only up to 24.6°.
Since we are in the ray optics picture, we can write:

$$R = \left| \frac{n_1 - n_2}{n_1 + n_2} \right|^2$$

$$T = 1 - R = 1 - \left[\frac{1-2.4}{1+2.4}\right]^2 \simeq 83\%$$

$$\eta = 83\% \ \frac{\Omega(\theta_c)}{4\pi} = 83\% \ \frac{1}{2}(1-\cos\theta_c)$$

$$\Omega(\theta_c) = \int_0^{2\pi} \mathrm{d}\phi \int_0^{\theta_c} \sin\theta \ d\theta = 2\pi(1-\cos\theta_c)$$

$$\eta = 83\% \ \frac{1}{2}(1-\cos\theta_c)$$

$$\eta = 83\% \ \frac{1}{2}(1-0.09) \simeq 0.83 \times 0.045 \simeq 3.7\%$$

- Would the apparent quantum yield change in the wave-optics picture?

  For a vertical dipole,

$$P(\theta,\phi) = P_0 \frac{3}{8\pi} \sin^2\theta$$

  here we assumed that the radiation is in free space.

$$\eta^v = \frac{3}{8\pi} \int_0^{2\pi} d\phi \int_0^{\theta_c} |t^p|^2 \ \sin\theta \ \mathrm{d}\theta$$

$$\eta^v = \frac{3}{4} \int_0^{\theta_c} |t^p|^2 \ \sin^3\theta \ \mathrm{d}\theta$$

$$\eta^v \ \simeq \ 83\% \ \frac{3}{4} \ \int_0^{\theta_c} (1-\cos^2\theta) \ \sin\theta \ \mathrm{d}\theta$$

$$\eta^v \ \simeq \ 83\% \ \frac{3}{4} \left[x - \frac{x^3}{3}\right]_{\cos\theta_c}^{1}$$

  Thus for th vertical dipole we get:

$$\eta^v \ \simeq \ 83\% \ \frac{3}{4} \left[(1-\cos\theta_c) + \frac{1}{3}(\cos^3\theta_c - 1)\right]$$

  For a horizontal dipole,

$$\eta^h = \frac{3}{4} \int_{\pi/2}^{\pi/2+\theta_c} \left|t^p\Big(\theta - \frac{\pi}{2}\Big)\right|^2 \ \sin^2\theta \ \sin\Big(\theta - \frac{\pi}{2}\Big) \ \mathrm{d}\theta$$

$$\eta^h = 83\% \ \frac{3}{4}\int_{\pi/2}^{\pi/2+\theta_c} (1-\cos^2\theta)(-\cos\theta)\ \mathrm{d}\theta$$

we can solve:

$$\int_{\pi/2}^{\pi/2+\theta_c} (\cos\theta)\ \mathrm{d}\theta \simeq (\cos\theta_c - 1)$$

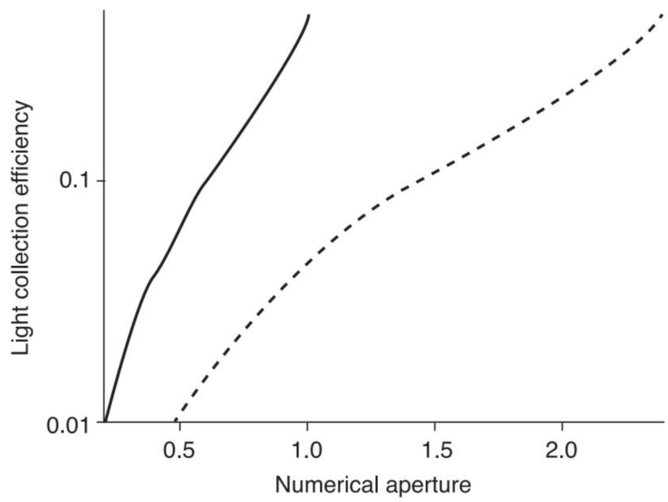
$$\int_{\pi/2}^{\pi/2+\theta_c} (\cos^3\theta)\ \mathrm{d}\theta = \int_{\pi/2}^{\pi/2+\theta_c} (1-\sin^2\theta)\ d\sin\theta$$

$$= \left[x - \frac{x^3}{3}\right]_{\sin\pi/2}^{\sin\pi/2+\theta_c} \ \simeq\ (\cos\theta_c - 1) - \frac{1}{3}(cos^3\theta_c - 1)$$

Thus for the horizontal dipole we get:

$$\eta^h = 83\% \ \frac{3}{4}\ \left[2\ (1-\cos\theta_c) + \frac{1}{3}(1-\cos^3\theta_c)\right]$$

- Comment on how the fluorescence collection efficiency varies as a function of the numerical aperture of the collection lens for a defect center surrounded by air and surrounded by diamond.



The collection efficiency is the fraction of photons emitted into a solid angle Ω given by $\frac{\Omega}{4\pi}$. The maximum angle at which the emitted photons to be collected is known as θ. The fraction F which is collected in this case will be :

$$F = \frac{1}{2}(1-\cos\theta) \tag{1}$$

If the photons are collected using a collection optics, lets consider a lens with a numerical aperture NA, the collection angle modified as follows:

$$\sin\theta = \frac{NA}{n}$$

where n is the refractive index of the medium surrounding the emitter. The fraction which is collected within the presence of a collection optics will be :

$$F = \frac{1}{2}\left[1 - \cos\left(\sin^{-1}\frac{NA}{n}\right)\right] \tag{2}$$

The figure above shows the fluorescence collection efficiency as a function of numerical aperture of the collection lens for a defect surrounded by air $n = 1$ (solid line) and surrounded by diamond, $n = 2.4$ (dashed line). The curves are plots of Eq. 2 with n = 1 and n = 2.4, respectively.

From the graph, it is clear that a high- NA objective lens is desirable, for maximising the optical signal. In the case of observing colour centres in bulk diamond it is cruicial, where the refraction at the diamond surface substantially reduces the solid angle over which fuorescence photons can be emitted if they are to couple into the objective lens. Hence, in this case having higher numerical apertures probably greater than 1 is desirable (eg: use of an oil immersion or solid immersion lens).

3 References

- Principles of Nano-Optics (Second edition) by Lukas Novotny
- Characterisation of single defects in diamond in the development of quantum devices by J. M. SMITH, University of Oxford, UK