Relationship between complex refractive index and absorption coeffcicient

In [1]:
```
%matplotlib inline
import math
import numpy as np
from __future__ import division
import matplotlib.pyplot as plt
import scipy.signal as sig
import scipy.constants as const
from IPython.display import display, Image, display_jpeg
import scipy.optimize as optim
```

Complex refractive index

$$N = n + i\kappa$$
$$E = E_0 e^{-i\omega t + iN\omega x/c} = E_0 e^{-i\omega t + i(n+i\kappa)\omega x/c} = E_0 e^{-\kappa\omega x/c} e^{-i\omega(t-nx/c)}$$

$$I \propto |E|^2 = E_0 2e^{-2\omega\kappa x/c}$$

$$I(x) \equiv I(0)e^{-\alpha x}$$

Therefore:

$$\alpha = \frac{2\omega\kappa}{c} = \frac{4\pi\kappa}{\lambda}$$

Permittivity and refractive index

At an optical frequency (~1e14Hz), a relative permittivity can be expressed as a complex number
$$\epsilon_r = \epsilon_r' + i\epsilon_r''$$

Relative permeability μ_r can be considered as the unity there. Maxwell's equation in a bulk matter can be simplified to the form
$$(N^2 - \epsilon_r)E = 0$$

Then $N^2 = \epsilon_r$ to allow non-zer E.

Now we substitute $N = n + i\kappa$ and $\epsilon_r = \epsilon_r' + i\epsilon_r''$. We obtain

$$\epsilon_r' = n^2 - \kappa^2$$
$$\epsilon_r'' = 2n\kappa$$

The special case if $\kappa = 0$ (transparent), $\epsilon_r = n^2$.

$$\alpha = \frac{2\pi\epsilon_r''}{n\lambda}$$
$$\kappa = \frac{\sqrt{-\epsilon_r' + |\epsilon|^2}}{\sqrt{2}}$$
$$n = \pm\frac{\sqrt{\epsilon_r' + |\epsilon|^2}}{\sqrt{2}}$$
$$\alpha = \frac{4\pi\sqrt{-\epsilon_r' + |\epsilon|^2}}{\lambda\sqrt{\epsilon_r' + |\epsilon|^2}}$$

Drude model

https://en.wikipedia.org/wiki/Drude_model (https://en.wikipedia.org/wiki/Drude_model)

Equation of motion for a free electron can be described as

$$m^* \frac{d^2u}{dt^2} + \frac{m^*}{\tau}\frac{du}{dt} = qE$$

where u, m^*, and τ are the position, effective mass, and scattering relaxation time of an electron.

The response of the electron against the external electric field E can be described in the frequency domain as usual

$$\tilde{u} = -\frac{q}{m^*}\frac{1}{\omega(\omega + i/\tau)}E$$

Polarization by a group of free electrons are described as

$$P = -Nqu$$

where N is the number density of the free electron. In frequency domain this becomes

$$\tilde{P} = Nq\tilde{u} = -\frac{Nq^2}{m^*}\frac{1}{\omega(\omega + i/\tau)}E$$

Therefore

$$\tilde{D} = \epsilon_0\epsilon_r\tilde{E} = \epsilon_0\tilde{E} + \tilde{P}$$

$$\epsilon_0\epsilon_r\tilde{E} = \epsilon_0\tilde{E} + -\frac{Nq^2}{m^*}\frac{1}{\omega(\omega + i/\tau)}E$$

We obtain

$$\epsilon_r = 1 - \frac{Nq^2}{m^*\epsilon_0}\frac{1}{\omega(\omega + i/\tau)}$$

$$\Longrightarrow \epsilon_r = 1 - \frac{\omega_p}{\omega(\omega + i/\tau)}, \quad \omega_p^2 \equiv \frac{Nq^2}{m^*\epsilon_0}$$

Here ω_p is the plasma frequency.

There is a relationship between the conductivity σ and the relaxation time τ as

$$\sigma = \frac{Nq^2}{m^*}\tau$$

or

$$\tau = \frac{m^*}{Nq^2}\sigma$$

Also the mobility is defined as

$$\sigma = Nq\mu$$

Therefore

$$\tau = \frac{m^*\mu}{q}$$

Now, we decompose the above relative permittivity ϵ_r with the real and imaginary parts ϵ_r' and ϵ_r''.

$$\epsilon_r = \epsilon_r' + i\epsilon_r''$$
$$= 1 - \frac{Nq^2}{m^*\epsilon_0}\frac{1}{\omega(\omega + i/\tau)}$$
$$\epsilon_r' = 1 - \frac{\omega_p^2}{\omega^2 + 1/\tau^2}$$
$$\epsilon_r'' = \frac{\omega_p^2}{\omega\tau(\omega^2 + 1/\tau^2)}$$

Note that there is some empirical technique to include detailed effects to match the refractive index at DC into the first term of ϵ_r'. i.e.

$$\epsilon_r' = \epsilon_c - \frac{\omega_p^2}{\omega^2 + 1/\tau^2}$$

Now we think about the absorption coeffcient α. We can substitue

$$\epsilon_r''$$

into the expression for α.

$$\alpha = \alpha = \frac{2\pi\epsilon_r''}{n\lambda}$$
$$= \frac{\omega_p^2}{nc\tau(\omega^2 + 1/\tau^2)}$$

τ for silicon is the order of $10^{-12} \sim 10^{-14} s$ while ω is $10^{15} rad/s$

In [2]:
```
me = 0.26*9.1e-31 # kg
q  = 1.6e-19 # C
mu = np.array([100, 10000]) # unit cm^2/V/s
mu_MKSA = mu/1e4
tau = me*mu_MKSA/q
display(tau) # unit: Hz
```

```
array([  1.47875000e-14,   1.47875000e-12])
```

Therefore, we can ignore the second term of the denominator.

$$\alpha = \frac{Nq^2}{m^*\epsilon_0 nc\omega^2\tau}$$
$$= \frac{q^3\lambda^2}{4\pi^2\epsilon_0 nc^3}\frac{N}{m^{*2}\mu}$$

This directly corresponds to the eq.5 in *Electrooptical Effects in Silicon*, R. A. Soref and B. R. Bennett, IEEE Journal of Quantum Electronics (ISSN 0018-9197), vol. QE-23, Jan. 1987, p. 123-129. http://dx.doi.org/10.1109/JQE.1987.1073206 (http://dx.doi.org/10.1109/JQE.1987.1073206)

In [3]:
```
# Free Carrier Absorption by Electron Carrier

nn = 1e13          # Carrier concentration 1/cm^3
nn_MKSA = nn*1e6 # => 1/m^3
me = 0.26*9.1e-31 # Effective mass kg
q  = 1.6e-19      # Electron charge C
lamb = 1550e-9    # Wavelength m
n  = 3.5          # Refractive index of Si 3.45@100K 3.47@293K for 1550nm
c  = 299792458    # Speed of light m
e0 = 8.9e-12      # Vacuum Permittivity F/m = C/(V m) = J/(V^2 m) = kg m/s^2/
V^2
mu = 1300         # Electron mobility unit cm^2/V/s
mu_MKSA = mu/1e4  #
pi = np.pi
alpha_MKSA = (pow(q,3)*pow(lamb,2)*nn_MKSA)/(4*pi*pi*e0*n*pow(c,3)*pow(me,2)*
mu_MKSA)
alpha = alpha_MKSA/100;
display(alpha) # unit: Hz
```

```
4.081037776913146e-06
```

In [4]:
```
# Free Carrier Absorption by Hole Carrier

nn = 1e13          # Carrier concentration 1/cm^3
nn_MKSA = nn*1e6 # => 1/m^3
me = 0.36*9.1e-31 # Effective mass kg
q  = 1.6e-19      # Electron charge C
lamb = 1550e-9    # Wavelength m
n  = 3.5          # Refractive index of Si 3.45@100K 3.47@293K for 1550nm
c  = 299792458    # Speed of light m
e0 = 8.9e-12      # Vacuum Permittivity F/m = C/(V m) = J/(V^2 m) = kg m/s^2/
V^2
mu = 460          # Hole mobility unit cm^2/V/s
mu_MKSA = mu/1e4  #
pi = np.pi
alpha_MKSA = (pow(q,3)*pow(lamb,2)*nn_MKSA)/(4*pi*pi*e0*n*pow(c,3)*pow(me,2)*
mu_MKSA)
alpha = alpha_MKSA/100;
display(alpha) # unit: 1/cm
```

```
6.015861510922024e-06
```

Temperature dependence

- Effective mass is not dependent on the temperature at low temperature. D. M. Riffe, "Temperature dependence of silicon carrier effective masses with application to femtosecond reflectivity measurements," J. Opt. Soc. Am. B 19, 1092-1100 (2002) http://dx.doi.org/10.1364/JOSAB.19.001092 (http://dx.doi.org/10.1364/JOSAB.19.001092)
- Mobility is a relatively strong function of the temperature. http://ecee.colorado.edu/~bart/book/transpor.htm (http://ecee.colorado.edu/~bart/book/transpor.htm) In general, the mobilities of the electon and hole goes up, because they are less scattered as the lattice vibration becomes quiet. Lightly doped silicon shows the electron mobility of 1400 and 11000+ cm^2/(V s) at 300K and 120K, respectively. The hole mobility of 470 and 3700 cm^2/(V s). https://www.pvlighthouse.com.au/calculators/mobility%20calculator/mobility%20calculator.aspx (https://www.pvlighthouse.com.au/calculators/mobility%20calculator/mobility%20calculator.aspx)

  The notable feature is that this dependence of the mobility on the temperature indicates that the resistivity goes down at low temperature. However, the free carrier absorption goes down. The resistivity is not a direct indicator of the free carrier absrption

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In [ ]:
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