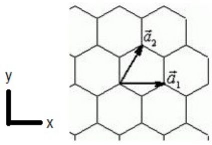
Exercise 6 (online: 05.06.2023. Return by: **Mo 12.06.2023 10:00**) **14P**

1. **Characterization of carbon nanotubes** 8P

   Use the following definition of the base vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ for carbon nanotubes:

   A set of carbon nanotubes (CNTs) exhibit the following chiral indices (n, m):
   (5,0), (6,3), (3,1) and (2,2).

   (a) Using the hexagonal lattice in Figure 1, sketch the respective vectors $\boldsymbol{C_k}$ for all CNTs in the set.(1P)

   (b) What is the geometrical type and electronic property of all CNTs in the set?(2P)

   (c) Calculate the diameters (in nm), circumferences (in nm) and chiral angles (in °) for all CNTs in the set.(3P)

   (d) Using the parameters $c_1 = 150\,\mathrm{nm/cm}$ and $c_2 = 30\,\mathrm{cm}^{-1}$ calculate the respective Raman shift $\Delta\tilde{\nu} = 1/\lambda_0 - 1/\lambda_1$ of the *radial breathing modes* (RBM) and sketch the corresponding (Stokes) range of the Raman spectrum of a mixture of the given nanotubes. Label the respective contributions.(2P)

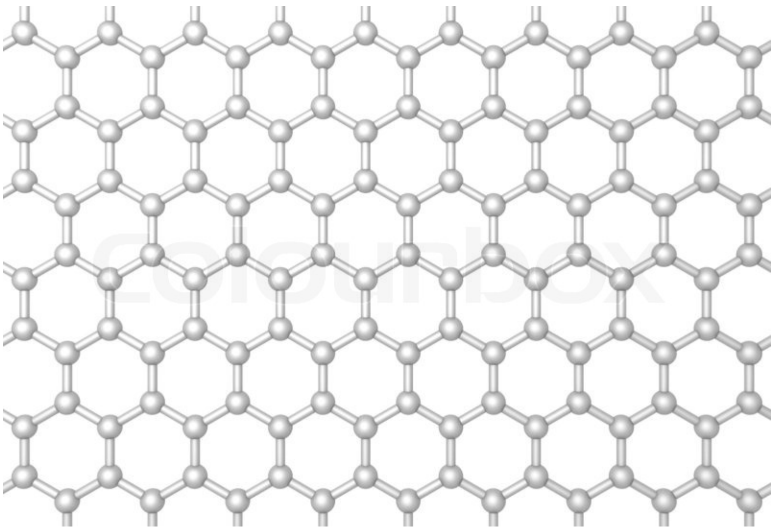


Figure 1: Hexagonal lattice.

2. **Dielectric function** 6P

An electrical field applied to a metal displaces the electrons by a vector of $\boldsymbol{x}$. The displacement results in a dipole moment $\boldsymbol{p} = -e\boldsymbol{x}$ and the polarization $\boldsymbol{P} = N\boldsymbol{p}$, where N is the electron density.

(a) For free electrons the Drude model can be applied according to

$$m_e \frac{d^2\boldsymbol{x}}{dt^2} + m_e \gamma \frac{d\boldsymbol{x}}{dt} = -e\boldsymbol{E_0}\, e^{-i\omega t}$$

with the effective electron mass m_e, the damping coefficient γ and the frequency of the applied field ω. Solve this equation using the Ansatz $\boldsymbol{x} = \boldsymbol{x}_0 e^{-i\omega t}$. Determine the dielectric function $\epsilon_D(\omega)$ (as a complex function with a separated real and imaginary part $\epsilon_D(\omega) = \epsilon_r + \mathrm{i}\epsilon_i$, with $\epsilon_r, \epsilon_i \in \mathbb{R}$) using $\boldsymbol{D} = \epsilon_0 \boldsymbol{E} + \boldsymbol{P} = \epsilon_0 \boldsymbol{E} - Ne\boldsymbol{x}$. Introduce the plasma frequency ω_p to the equation.(2P)

(b) For bound particles the description by the Drude model is insufficient. To take into account the contribution of bound electrons, an extended equation of motion with a restoring force can be formulated:

$$m_e^* \frac{d^2\boldsymbol{x}}{dt^2} + m_e^* \Gamma \frac{d\boldsymbol{x}}{dt} + \alpha \boldsymbol{x} = -e\boldsymbol{E_0} e^{-i\omega t}$$

with the effective electron mass m_e^*, damping Γ and the spring constant α of the potential that keeps the electron in place. Solve the equation analogous to (a) and determine the complex dielectric function $\epsilon_B(\omega) = \epsilon_r + \mathrm{i}\epsilon_i$. In this case use the modified plasma frequency $\bar{\omega}_p$ with $\bar{n}$ the density of bound electrons, the effective mass m_e^* and $\omega_0^2 = \alpha/m_e^*$.(2P)

(c) Plot the real and imaginary parts of the dielectric functions ϵ_D and ϵ_B for gold over the wavelength λ in nm with the parameters below as well as $\hbar\omega_0 = 2.07\,\mathrm{eV}$. Create one combined plot with λ from $400\,\mathrm{nm}$ to $800\,\mathrm{nm}$ (visible light) and $\epsilon_{D/B}(\hbar\omega)$ from -40 to 10. Use for gold in the Drude model: plasma frequency $\hbar\omega_p = 8.95\,\mathrm{eV}$ and damping coefficient $\hbar\gamma = 65.8\,\mathrm{meV}$; and for bound electrons: plasma frequency $\hbar\bar{\omega}_p = 2.96\,\mathrm{eV}$ and damping coefficient $\hbar\Gamma = 0.59\,\mathrm{eV}$. (2P)

(d) Briefly describe the characteristic behaviour of the real and imaginary parts of ϵ_D and ϵ_B. What is the physical interpretation of this behaviour (also taking into account that the refractive index $n = \sqrt{\epsilon}$)? (1P, Optional)