Introduction to Physics of Nanoparticles and Nano structures

Part I: Physics of Nanoparticles **Questions on Module 3**

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1. *Lorentz Oscillator model :* Consider the motion of an electron of charge $-e$ bound to an atom or ion or a molecule by a damped harmonic force of frequency ω_o and damping constant γ under the influence of an external electric field $\vec{E}(\vec{x}, t)$ having a time dependence of the form $e^{-i\omega t}$. Assuming that the difference between the external field and the local electric field is negligble, show that the dielectric permittivity $\varepsilon(\omega)$ for a system of N such atoms or ions or molecules is given by

$$\frac{\varepsilon(\omega)}{\varepsilon_o} = 1 + \sum_j \frac{\omega_{pj}^2}{\omega_j^2 - \omega^2 - i\omega\gamma_j},$$

where $\omega_{pj}^2 = Ne^2 f_j/(m\varepsilon_o)$, with f_j denoting the oscillator strength and ε_o the free-space permittivity.

2. Consider the single oscillator model,

$$\frac{\varepsilon(\omega)}{\varepsilon_o} = 1 + \frac{\omega_{po}^2}{\omega_o^2 - \omega^2 - i\omega\gamma},$$

where $\omega_{po}^2 = Ne^2/(m\varepsilon_o)$, and let $\varepsilon(\omega)/\varepsilon_o = \epsilon'(\omega) + i\epsilon''(\omega)$.

   (a) Show that
$$\epsilon''(\omega = \omega_o \pm \gamma/2) = \epsilon''_{max}/2.$$

   (b) Show that
$$\epsilon'_{max} = 1 + \epsilon''_{max}/2, \qquad \text{and} \quad \epsilon'_{min} = 1 - \epsilon''_{max}/2,$$

   (c) Establish the Kramer-Kronig relation between $\epsilon'(\omega)$ and $\epsilon''(\omega)$.

   (d) Show that
$$\omega_{po}^2 = \frac{2}{\pi}\int_0^\infty \epsilon''(\omega_1)\omega_1 d\omega_1, \qquad (\mathrm{f-sum\,rule}).$$

   (e) Show that if $\sqrt{\epsilon(\omega)} = n(\omega) + ik(\omega)$ and $\alpha(\omega)$ is the absorption coefficient, then for $\gamma \ll \omega_o$,
$$N = \frac{mcn(\omega_o)}{2\pi^2 e^2}\int_0^\infty \alpha(\omega_1)d\omega_1.$$

3. A single oscillator model accounting for lattice vibration in ionic crytals is,

$$\epsilon(\omega) = \epsilon_{oe} + \frac{\omega_{po}^2}{\omega_t^2 - \omega^2 - i\omega\gamma},$$

where ϵ_{oe} is the electronic contribution from high frequency excitations, and ω_t is the frequency corresponding to the transverse optical mode.

(a) If $\epsilon'(\omega \ll \omega_t) = \epsilon_{0v}$, $\gamma \ll \omega_t$ and $\epsilon'(\omega = \omega_l) = 0$, then show that

$$\frac{\omega_l^2}{\omega_t^2} = \frac{\epsilon_{ov}}{\epsilon_{oe}}. \qquad \text{(Lyddane – Sachs – Teller relation)}$$

(b) Show that

$$\epsilon'(\omega) = \epsilon_{oe}\left[1 + \frac{\omega_l^2 - \omega_t^2}{\omega_t^2 - \omega^2}\right].$$

(c) If for a material, $\omega_t = 800 cm^{-1}$, $\gamma \ll \omega_t$, $\omega_{po}^2 = 2.1 \times 10^6 cm^{-2}$, and $\epsilon_{oe} \approx 7$, then find approximately the width (in cm^{-1}) of the frequency window in which the reflectance of the material at normal incidence is close to unity.

4. Consider a two oscillator model for lattice vibration in a crystal, described by

$$\epsilon(\omega) = \epsilon_{oe} + \frac{\omega_{p1}^2}{\omega_1^2 - \omega^2 - i\omega\gamma_1} + \frac{\omega_{p2}^2}{\omega_2^2 - \omega^2 - i\omega\gamma_2}.$$

(a) If $\gamma_1 \ll \omega_1$ and $\gamma_2 \ll \omega_2$, then determine ω for which ϵ' vanishes, *i.e.*, $\epsilon'(\omega_l) = 0$.

(b) For a material, $\epsilon_{oe} \approx 3$, $\omega_1 = 400 cm^{-1}$, $\gamma_1 \ll \omega_1$, $\omega_{p1}^2/\omega_1^2 = 6.6$, $\omega_2 = 640 cm^{-1}$, $\gamma_2 \ll \omega_2$, $\omega_{p2}^2/\omega_2^2 = 0.045$. Estimate $\omega_l - \omega_1$ in cm^{-1}.

5. In a anistotropic solid the dielctric function is a tensor and in diagonal form, is given by

$$\overleftrightarrow{\epsilon} = \begin{bmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_3 \end{bmatrix},$$

where ϵ_1, ϵ_2, and ϵ_3 are the principal dielectric functions. Consider the propagation of plane wave $\vec{E}_o e^{i(\vec{q}\cdot\vec{x} - \omega t)}$ in the medium. If the wave propagates along the third principal axis (along ϵ_3, taken as z-axis), then show that the wave is transverse and the wave can propagate without a change in polarization if it is either x-polarized or y-polarized; find the wave vector in each case of polarization.

6. *Drude model:* In metals, electrons are free and in the single oscillator model, $\omega_o = 0$, giving the dielectric function for metal as

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)},$$

where ω_p is the plasma frequency given by $\omega_p^2 = Ne^2/(m\varepsilon_o)$, with N denoting the free electron density.

(a) Find the reflectance at normal incidence in the frequency range 0 to ω_p, assuming $\gamma \ll \omega_p$.

(b) Show that the dielctric function gives a static conductivity σ_{static} consistent with simple collision approach to electron transport.

(c) Compute ω_p (in $\sec^{-1}$) and the corresponding wavelength λ_p for a metal with electron density $N = 10^{22}\, cm^{-3}$.

7. *Debye relaxation model :* In polar materials comprising of molecules with permanent dipole moments, the dipoles can relax through rotational motion, which determine the low frequency (usually in the microwave range) dielectric function of the material. Debye showed that the polarization in response of such a material to a time-harmonic field $E_o e^{-i\omega t}$ is

$$P(t) = \varepsilon_o \chi_{0v}\, E_o\, e^{-i\omega t} + \varepsilon_o(\chi_{0d} - \chi_{0v}) \int_{-\infty}^{t} E_o\, e^{-i\omega t_1} \frac{d}{dt_1}[e^{-(t-t_1)/\tau}]dt_1,$$

where χ_{0v} is the susceptibility at low frequencies (low compared with chracteristic lattice vibrational frequencies, which in turn are low compared with electronic transition frequencies), χ_{0d} is the static dipolar susceptibility, and τ is the relaxation time.

(a) Show that above leads the low frequency susceptibility

$$\chi(\omega) = \chi_{0v} + \frac{\Delta}{1 - i\omega\tau}, \qquad \Delta = \chi_{0d} - \chi_{0v}$$

(b) Find the real and imaginary parts (ϵ' and ϵ'') of the dielectric function corresonding to the above susceptibilty and the find the frequency ω_o at which ϵ'' is maximum, and $\epsilon''(\omega_o)$.

(c) For a polar liquid, the maximum in ϵ'' occurs at frequency $\omega_o = 1.25 Hz$, and $\epsilon''(\omega_o) \approx 36$. If $\epsilon_{0v} = 5.3$, then compute the values of τ and ϵ_{0d}.

(d) Debye showed that the relaxtion time for a sphere of radius a in fluid of viscosity η is

$$\tau = \frac{4\pi\eta a^3}{k_B T},$$

where T is the absolute temperature and k_B is the Boltzman constant. If for a polar liquid, T=300 K, and corresponding value of η is 0.01 gm/cm-sec, then taking $a = 10^{-8}\, cm$, compute the value of τ.

(e) Show that for a single relaxation time, the plot of ϵ'' versus ϵ' (*Cole-Cole plot*) is a semicircle centered on the ϵ' axis at $(\epsilon_{0d} + \epsilon_{0v})/2$ with radius $(\epsilon_{0d} - \epsilon_{0v})/2$.

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