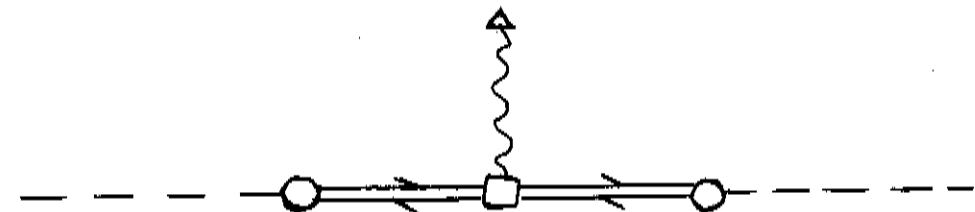


**answer to question 1(a)**

Explain why the  $G$  band and  $G'$  band appear in the Raman spectra of a perfect graphite crystal (HOPG - highly oriented pyrolytic graphite) while the  $D$  band is observed only on defective graphitic materials.

Due to momentum conservation. Since the light has large wavelength ( $\lambda \sim 5000 \text{ \AA}$ ) compared to the lattice unit cell dimensions ( $a \sim \text{few \AA}$ ), the wavevector of light ( $k = 2\pi/\lambda$ ) is close to the center of the Brillouin zone ( $q \sim 0$ ). Only phonons with ( $q \sim 0$ ) can be involved in a first order Raman scattering process that conserve momentum. Raman scattering by phonons with  $q \gg 0$  can occur in a second-order process, where two phonons with  $q$  and  $-q$  scatter the same electron, thus conserving momentum. This is the case for the  $G'$  band. The  $D$  band involves only one phonon with  $q \gg 0$ , and elastic scattering by a defect brings the electron to the original  $k$  vector, so that momentum is conserved.

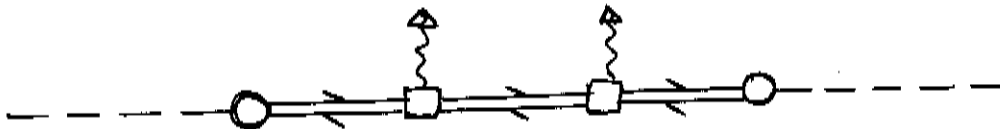
G band



D band



G' band



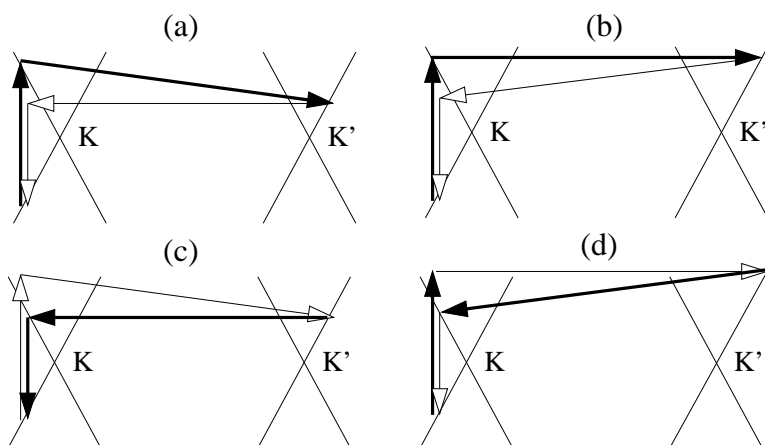
**answer to problem 1(c)**

Four scattering processes must be considered:

resonance with    first scattering    second scattering

incident	elastic	inelastic
incident	inelastic	elastic
scattered	elastic	inelastic
scattered	inelastic	elastic

The phonons involved on the Raman process where inelastic scattering occurs before the elastic scattering [figs.(a) and (c)] are different from the phonons involved on the Raman process where elastic scattering occurs before the inelastic scattering [figs.(b) and (d)]. Therefore, two peaks are expected to appear in the D-band spectra.



$$\textcircled{3} \quad R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} = \frac{n^2 + k^2 + 1 - 2n}{n^2 + k^2 + 1 + 2n} \quad \alpha = \frac{2\omega}{c} k$$

$$\begin{cases} n^2 - k^2 = \varepsilon_1 = \varepsilon_1^0 + \varepsilon_1^1 E \\ 2nk = \varepsilon_2 = \varepsilon_2^0 + \varepsilon_2^1 E \end{cases}$$

$$4n^2 k^2 = 4n^2 (n^2 - \varepsilon_1) = \varepsilon_2^2$$

$$n^4 - \varepsilon_1 n^2 - \frac{\varepsilon_2^2}{4} = 0$$

$$n^2 = \frac{\varepsilon_1}{2} \pm \frac{1}{2} \sqrt{\varepsilon_1^2 + \varepsilon_2^2} = \frac{1}{2} (\sqrt{\varepsilon_1^2 + \varepsilon_2^2} + \varepsilon_1)$$

not physical

$$k^2 = n^2 - \varepsilon_1 = \frac{1}{2} (\sqrt{\varepsilon_1^2 + \varepsilon_2^2} - \varepsilon_1)$$

$$\Delta R = \frac{\sqrt{\varepsilon_1^2 + \varepsilon_2^2} + 1 - \sqrt{2} \sqrt{\varepsilon_1^2 + \varepsilon_2^2} + \varepsilon_1}{\sqrt{\varepsilon_1^2 + \varepsilon_2^2} + 1 + \sqrt{2} \sqrt{\varepsilon_1^2 + \varepsilon_2^2} + \varepsilon_1} - \frac{\sqrt{\varepsilon_1^2 + \varepsilon_2^2} + 1 - \sqrt{2} \sqrt{\varepsilon_1^2 + \varepsilon_2^2} + \varepsilon_1}{\sqrt{\varepsilon_1^2 + \varepsilon_2^2} + 1 + \sqrt{2} \sqrt{\varepsilon_1^2 + \varepsilon_2^2} + \varepsilon_1}$$

$$\Delta \alpha = \frac{\sqrt{2}\omega}{c} \left[ \sqrt{\varepsilon_1^2 + \varepsilon_2^2} - \varepsilon_1 - \sqrt{\varepsilon_1^2 + \varepsilon_2^2} - \varepsilon_1 \right]$$

$$\Delta R \propto \frac{1}{\sqrt{E}} \quad \Delta \alpha \propto \sqrt{E} \quad \text{at high fields}$$

4 (a)

Flux · duration · molecular area = coverage

Flux · average momentum transfer = pressure

$$p [\text{Pascal}] = \frac{\langle \Delta \bar{p} \rangle \cdot 0.1}{1 \text{ hr} \cdot \pi (3.4)^2 \text{ \AA}^2} = \langle \Delta \bar{p} \rangle \cdot 7.65 \cdot 10^{13} \text{ m}^{-2} \text{ sec}^{-1}$$

$$\langle \Delta \bar{p} \rangle = \int_0^{\pi/2} 2 \sqrt{\langle p^2 \rangle} \sin \theta \, d\theta \Big/ \frac{\pi}{2} = \frac{4}{\pi} \sqrt{\langle p^2 \rangle}$$

$$\langle E_{\text{kin}} \rangle = \frac{\langle p^2 \rangle}{2M_{O_2}} = \frac{3}{2} kT$$

$$\Downarrow$$

$$\begin{aligned} \langle \Delta \bar{p} \rangle &= \frac{4}{\pi} \sqrt{3M_{O_2} kT} = \frac{4}{\pi} \left( 3 \cdot \frac{0.032}{6.0 \cdot 10^{-23}} \cdot 1.38 \cdot 10^{-23} T \right)^{1/2} \\ &= \frac{4}{\pi} \cdot 1.5 \cdot 10^{-24} T^{1/2} \text{ kg} \cdot \frac{\text{m}}{\text{sec}} \end{aligned}$$

$$p [\text{Pascal}] = 1.45 \cdot 10^{-10} T^{1/2} \text{ kg m}^{-1} \text{ sec}^{-2}$$

$$p [\text{torr}] = 7.5 \cdot 10^{-3} p [\text{Pascal}] = 1.1 \cdot 10^{-12} T^{1/2}$$

$$p(300\text{K}) = 2 \cdot 10^{-11} \text{ torr}$$

$$p(77\text{K}) = 8.7 \cdot 10^{-12} \text{ torr}$$

4 (b)

$$n = \frac{2}{(2\pi)^3} \cdot \frac{4}{3} \pi k_F^3$$

$$\frac{n_{\text{compound}}}{n_K} = \frac{E_{F \text{ compound}}^{3/2}}{E_{F K}^{3/2}} = \left(\frac{1.25}{2}\right)^{3/2} = 0.484$$

In K 50% of the band is occupied, so in the compound 24.7% is.

(c) While the sample composition is 50%-50% Cu/Ni, lattice positions at the surface are more likely to be occupied by Cu atoms.

$$(d) \quad J_T = \frac{e^2}{\hbar} \cdot \frac{\kappa}{4\pi^2 z} V_T \exp(-2\kappa z)$$

$$\kappa = (2m\phi)^{1/2} / \hbar = 0.512 [\text{\AA}^{-1} \text{eV}^{-1/2}] \cdot \phi^{1/2} = 1.16 \text{\AA}^{-1}$$

$$V_T = V - J_T \cdot \rho \cdot l$$

$$J_T = \frac{e^2}{\hbar} \cdot 1.4 \cdot 10^{-2} \text{\AA}^{-2} \cdot (V - J_T \rho l) \cdot 1.18 \cdot 10^{-2}$$

$$J_T = \frac{e^2 V}{\hbar} \cdot 1.66 \cdot 10^{-4} \text{\AA}^{-2} \cdot \left[ 1 + \frac{e^2}{\hbar} \rho l \cdot 1.66 \cdot 10^{-4} \text{\AA}^{-2} \right]^{-1}$$

$$= 2 \cdot 10^{-7} \frac{\text{A}}{\text{\AA}^2} [1 + 40000]^{-1}$$

$$= 5 \cdot 10^{-12} \text{ A/\AA}^2$$