



भारतीय प्रौद्योगिकी संस्थान पटना
Indian Institute of Technology Patna
End Semester Examination (End-Sem) (Aug-Nov-2011)

COURSE NO: PH401

Duration: 3 hours

COURSE TITLE: Introduction to Nanomaterials

Full Marks: 50

1. Answer All the questions:

[5x2=10]

- Plot the energy versus DOS (Density of States) for (a) (9,9) metallic conducting CNT (Carbon Nanotubes) and (b) (11,7) semiconducting CNT.
- What is the difference between energy band gaps of two carbon nanotubes with diameters 15Å and 25Å.
- Discuss the mechanical and thermal properties of carbon nanotube.
- Discuss the three common connectivity schemes to prepare nanocomposites.
- What are the advantages to put CNTs into polymers?

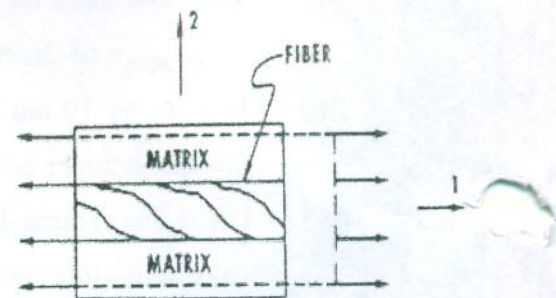
2. Answer all the questions:

[10x3=30]

- A liquid drop has contact angle $\theta = 45^\circ$. Find out the surface energy γ_{sl} ($\gamma_{lv} = 0.042 \text{ Jm}^{-2}$ and $\gamma_{sv} = -0.061 \text{ Jm}^{-2}$. Find out the wetting parameter S and discuss your result.
- Why can trees be no longer than 130m (427ft)? Justify your answer by taking $\gamma_{\text{water-xylem}} = 64.2 \text{ mN.m}^{-1}$ and contact angle $= 0^\circ$.
- How many 10 nm nanocubes are required to produce the same surface area as a one cubic meter cube? How much volume do they occupy?
- Using the Young-Laplace equation, compare ΔP for ideal spherical bubbles of 1mm and 10nm in water at ambient pressure? How you compare nanomaterials efficiency with bulk material from this result. [$\gamma_{\text{water}} = 0.0728 \text{ N/m}$]
- Calculate the change in ΔE_s energy when 4 nanoparticles of Au (gold) with $d = 20 \text{ nm}$ ($\gamma = 0.54 \text{ N/m}$) combine to form one large drop (diameter = D). Assume isothermal conditions.

P.T.O

- (vi) In an experiment nano droplets increase its size from 5nm to 50nm in 5minutes (thermo dynamical conditions are same throughout the experiment). What is the rate of change of free energy (ΔG)? [Free energy per unit volume (ΔG_v) = 0.041Joule/m³ and surface tension of droplet (γ) = 0.074Joule/m²].
- (vii) Discuss MEMS vs. Integrated Circuits (IC).
- (viii) Write short note on coulomb blockade. How it is applied to nanotransistors i.e. single electron transistor? Plot the V-I characteristic of nanoconductors. Two Cu nanoparticles of diameter 2nm each combined and make a bigger nanoparticle. What is the net resistance of bigger Cu nanoparticle if the individual Cu nanoparticle (2nm) resistance is 4m Ω .
- (ix) Discuss the advantages and disadvantages of Montecarlo (MC) and Molecular Dynamics (MD) simulations for nanomaterials.
- (x) Consider a linear butadiene molecule. What is the length of the box? Calculate the energy of an electron confined in this molecular box? What is the expected absorption of butadiene CH₂=C-C=CH₂? [m_p = 1.67X10⁻²⁷kg, m_e = 9.1X10⁻³¹kg and h = 6.626 \times 10⁻³⁴ J.s . What do you mean by zero dimensional materials?
3. A unidirectional carbon/epoxy lamina with E_f = 220 GPa, E_m = 2 GPa, and V_f = 0.55. (i) Estimate the value of the composite longitudinal modulus E_L , (ii) Estimate the value of the composite transverse modulus E_2 . (iii) If fiber Poisson's ratio n_f = 0.25 and n_m = 0.35, find the lamina Poisson's ratio n_{L2} .?
- (v) One can increase E_m by reinforcing randomly carbon nanotubes. For example, 5% and 25% volume fraction of V_{NT} can modify the E_m to 4GPa and 10GPa respectively. Can E_L increases upto stiffness of aluminum (E = 69 GPa) by reinforcing carbon nanotube into the matrix. [4]
4. Discuss the 8 steps of MEMS fabrication. How can MEMS cantilever beams being used as biosensors, temperature sensors, charge sensors, pressure sensor and magnetic sensors? Can one MEMS device integrate all the above sensors? [6]



-----XXXXXX-----

BEST OF LUCK