End-Spring Semester Examination, 2017

Mechanical Engineering Department

Indian Institute of Technology, Kharagpur

Subject: Micromechanics and Nanomechanics (ME 60432)

Full Marks: 50 Time : 3 Hrs

Answer all questions and assume reasonably wherever necessary.

1. Using the Differential scheme derive a micromechanics model of a heterogeneous medium with one inhomogeneity as follows:

$$\frac{d[C]}{dv_1} = \frac{1}{1-v_1}\left([C_1]-[C]\right)[A_1([C])]$$

in which $[C]$ is the effective elastic constant matrix of the medium, $[C_1]$ is the elastic constant matrix of the inhomogeneity, v_1 is the volume fraction of the inhomogeneity and $[A]$ is the strain concentration tensor. (10)

2. Show that the effective Young's modulus of a one-dimensional bar having periodic microstructures can be estimated by the asymptotic homogenization method as follows:

$$E_{eff} = \left(\frac{1}{d}\int_{y_0}^{y_0+d}\frac{d\tilde{y}}{E(\tilde{y})}\right)^{-1}$$

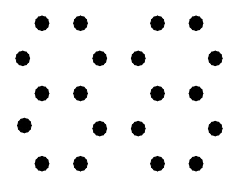
in which d is the periodicity of the microstructure and $E(\tilde{y})$ is the periodic function with periodicity d representing the Young's modulus at any point in the bar at microscale. (10)

3. (a) In a system of atoms, the pair-wise interaction potential energy between any two atoms is given by the Lennard-Jone potential (V_{LJ}) as

$$V_{LJ}(r) = -\frac{A}{r^6} + \frac{B}{r^{12}}$$

where the constants A and B are the strengths of the attractive and the repulsive interactions, respectively and r is the distance between the atoms. Determine the equilibrium distance and the binding energy between the atoms. (3+3)

(b) For the lattice structure shown in the Figure aside, draw the Wigner-Seitz primitive cell. Considering in-plane translational degrees of freedom only, write the potential energy of the atom of the cell and derive the stiffness matrices given by $[K_{n,n'}]$ corresponding to this atom. (2+4+6)



4. (a) What is the difference between an "arm chair" **CNT** and a "zig zag" **CNT** ? Determine the diameter of an (m, n) **SWCNT**. (1+3)

(b) For continuum modeling of a **CNT**, the covalent bonds between the atoms can be treated as the equivalent bars or beams. Derive the sectional properties of these equivalent bars or beams in terms of atomic force constants. (6)

(c) Briefly discuss how the interface between the **CNT** and epoxy matrix of a nanocomposite can be modeled as an equivalent interphase layer. (2)