I. PROBLEM SESSION 3

A. Problem 3.1

Cohesive energy of bcc and fcc neon:
Using the Lennard Jones potential, calculate the ratio of the cohesive energies of neon in the bcc and fcc structures ($Ans = 0.958$). The lattice sums for the bcc structure are $\sum_j' p_{ij}^{-12} = 9.11418$ $\sum_j' p_{ij}^{-6} = 12.2533$.

B. Problem 3.2

Solid molecular hydrogen:
For H_2 one finds from measurements on the gas that the Lennard-Jones parameters are $\epsilon = 50 * 10^{-16}$erg and $\sigma = 2.96\AA$. Find the cohesive energy in kJ per mole of H_2, do the calculation for an fcc structure. Treat each H_2 molecule as a sphere.
The observed cohesive energy is $0.751 kJ/mol$, much less than calculated form our simple model. Thus quantum corrections should be important.

C. Problem 3.3

-Recall the definition of the stress tensor,$\hat{\sigma} = \sigma_{ij}$.
-How can the force acting on a unit area with normal vector $\vec{n}$ be expressed through $\hat{\sigma}$.
-Let us rotate the coordinate frame by an angle α in the xy plane. Find how the stress tensor $\hat{\sigma}$ is transformed.
-Show that the trace $(\sum_i \sigma_{ii})$ of this tensor has not changed.
Define the deformation tensor ϵ_{ik} through the displacement vector $\vec{u}(\vec{r})$. Why does only the symmetric component enter? What is the physical meaning of $(\delta u_i/\delta x_k - \delta u_k/\delta x_i)$?

D. Problem 3.4

-Recall the general relationship between the strain tensor ϵ_{ik}, and the stress tensor, σ_{ik}.
-How does this relation look for an elastic medium? How many elastic constants enter this relationship?
-Explain the meaning of the Young's modulus E, the shear modulus, G, and the Poisson ratio, v. How can these quantities be measured experimentally?