MSE 102, Fall 2011 Midterm #2

Write your name here: ______________________________________

Instructions:

- Answer all questions to the best of your abilities. Be sure to write legibly and state your answers clearly.
- The point values for each question are indicated.
- You are not allowed to use notes, friends, phones, etc.
- You can use calculators.
- There are a total of 100 points.
- Feel free to ask questions, but only for clarification purposes.

(1a) [10 POINTS] Suppose that the interaction between two atoms is given by the Lennard-Jones potential:

$$V(d) = 4\varepsilon\left[\left(\frac{\sigma}{d}\right)^{12} - \left(\frac{\sigma}{d}\right)^{6}\right] \quad .$$

Choose $\varepsilon = 4.0$ eV, and $\sigma = 2.0$ Å. Consider a crystal with one atom per unit cell and primitive lattice vectors:

$$\mathbf{a} = \frac{\eta}{2}\mathbf{e}_x + \frac{\eta}{2}\mathbf{e}_y$$

$$\mathbf{b} = \frac{\eta}{2}\mathbf{e}_x - \frac{\eta}{2}\mathbf{e}_y$$

Find the equilibrium lattice parameter η for the crystal. Be sure to give the proper units. The following sums will be useful.

$\sum_{u=-\infty}^{\infty}\sum_{v=-\infty}^{\infty}\left(\frac{1}{u^2+v^2}\right)^3 = 4.65891$ and $\sum_{u=-\infty}^{\infty}\sum_{v=-\infty}^{\infty}\left(\frac{1}{u^2+v^2}\right)^6 = 4.06402$. (The sums exclude the singular terms.)

(1b) [10 POINTS] Evaluate the total energy per atom of the crystal at the equilibrium lattice parameter you calculated. Again, be sure to include the units in your final answer.

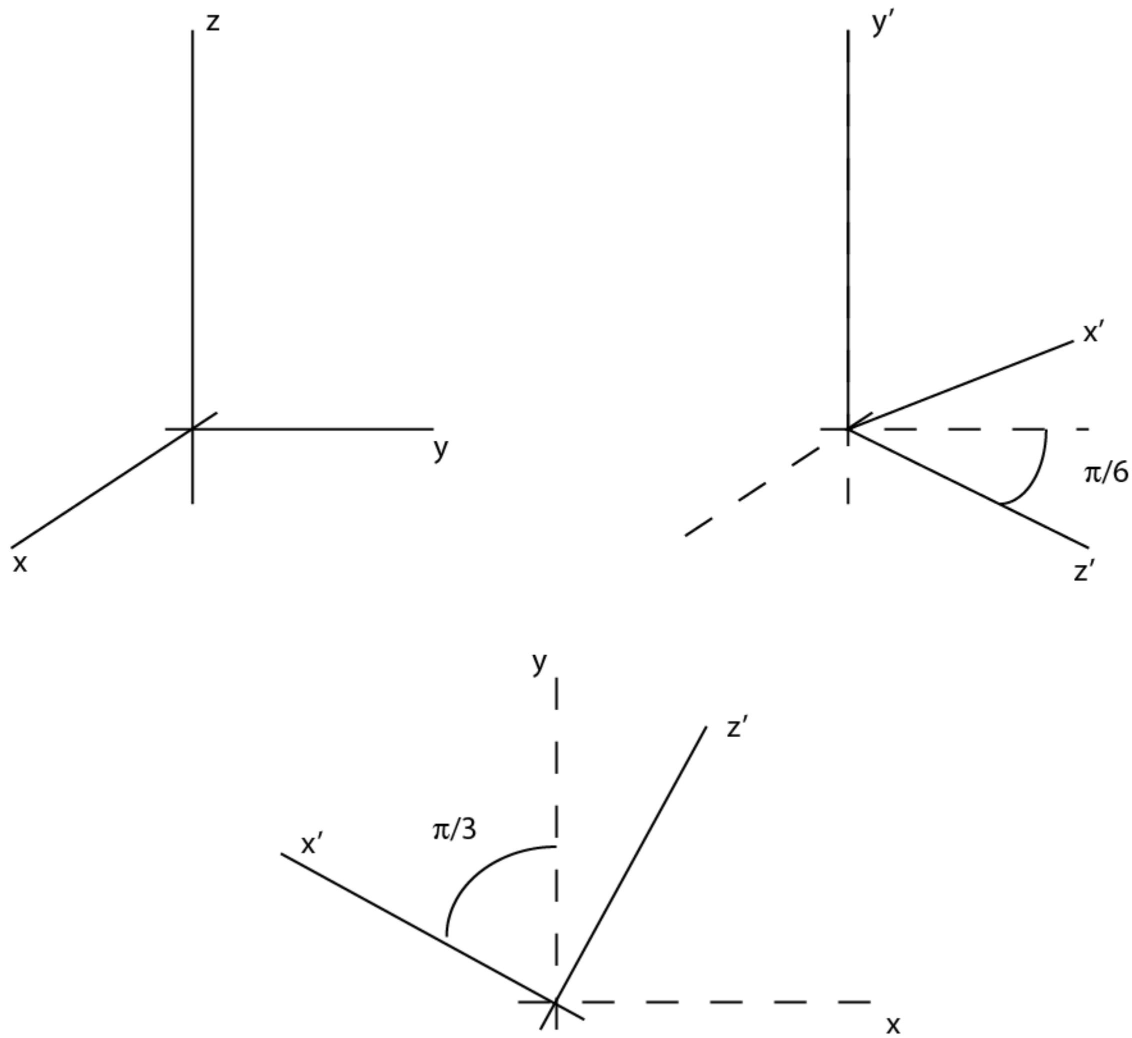
(1c) [5 POINTS] The 2-D bulk modulus, B, of this material can be defined according to:

$$B = A\frac{\partial^2 E}{\partial A^2}.$$

with E the energy per atom, and A the area per atom. Evaluate the 2-D bulk modulus for this material. Be sure to report the units for your modulus.

(2) [5 POINTS] Prove that if a 2^{nd} rank tensor is symmetric in the unprimed frame, that it will be symmetric in the primed frame.

(3) Two coordinate systems are defined as shown in the figure.



(3a) [10 POINTS] Give the transformation matrix relating the two coordinate systems.

(3b) [10 POINTS] The conductivity tensor in the unprimed frame is given by:

$$\sigma = \begin{bmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \beta \end{bmatrix}.$$

Express all of the components of the conductivity in the primed frame in terms of the values of α and β. (You can use the fact that the transformation of a symmetric 2^{nd} rank tensor yields a symmetric 2^{nd} rank tensor.)

(4) [10 POINTS] A cubic material is strained according to the following strain tensor:

$$\varepsilon = \begin{bmatrix} \alpha & \gamma & 0 \\ \gamma & \alpha & 0 \\ 0 & 0 & \alpha \end{bmatrix}.$$

Give the associated stress tensor in terms of the parameters α and γ and the elastic constants C_{11}, C_{12}, and C_{44}.

(5) [10 POINTS] A crystal has a two-fold axis of symmetry along its x_3-axis. The piezoelectric tensor is defined to be d_{ijk}. What, if anything, does the two-fold axis of symmetry imply for the values of d_{111}, d_{222} and d_{123}? Justify your answer.

(6) An electron bound to a hydrogen atom is described by the wavefunction:5

$$\Psi(\mathbf{r},t) = \frac{1}{\sqrt{5}}\exp\left(\frac{-iE_3t}{\hbar}\right)\psi_{310}(\mathbf{r}) - i\frac{2}{\sqrt{5}}\exp\left(\frac{-iE_3t}{\hbar}\right)\psi_{32-1}(\mathbf{r}),$$

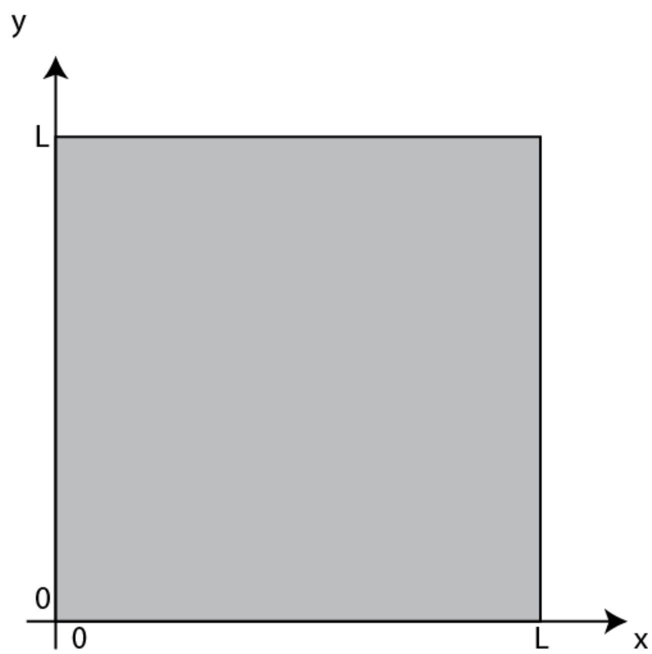
with $\psi_{nlm}(\mathbf{r})$ an eigenfunction of the Hamiltonian, $\hat{H}$, squared angular momentum, $\hat{L}^2$, and z-component of the angular momentum, $\hat{L}_z$.

(6a) [5 POINTS] Give the expectation value of the z-component of the angular momentum, $\hat{L}_z$, for the electron.

(6b) [5 POINTS] Give the expectation value of the total energy.

(6c) [5 POINTS] Give the expectation value of the angular momentum squared, $\hat{L}^2$.

(7) A particle of mass m is confined to the two-dimensional sheet sketched below. That is, the potential everywhere in the shaded region is identically zero, and the potential outside the shaded region is infinite.



(7a) [5 POINTS] Within the sheet, the time independent Schrödinger equation can be written:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\psi(x,y)=E\psi(x,y).$$

Assume that the solution to the equation can be written as a product of two functions:

$$\psi(x,y)=X(x)Y(y).$$

Using this assumed form, derive the differential equations that must be satisfied by $X(x)$ and $Y(y)$. Also, give the boundary conditions governing the solutions to these equations.

(7b) [10 POINTS] The solution to the equation can be written:

$$\psi(x,y) = \frac{2}{L}\sin\left(\frac{n_x\pi}{L}x\right)\sin\left(\frac{n_y\pi}{L}x\right)$$

with n_x and n_y integers greater than or equal to 1. Substitute this expression into the time independent Schrödinger equation and obtain an expression for the energy eigenvalues. What are the three lowest (unique) values that one might measure for the energy of this particle?