Homework 4
Due 25 October 2018
The numbers following each question give the approximate percentage of marks allocated to that question.

1. Use the reciprocal metric tensor again to calculate the angle between (112) and (431) planes in a monoclinic unit cell with lattice constants \( a = 1 \text{ Å}, \ b = 2 \text{ Å}, \ c = 4 \text{ Å}, \) \( \beta = 95^\circ \). You can use dSpace to check your answer:
   http://coen.boisestate.edu/rickubic/files/2012/05/dSpace.exe

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2. Consult the International Tables (https://it.iucr.org/Ab/) for space group P3. Inserting a single atom into the 1a site in this space group results in a site point symmetry which is not “3…” as listed.

a. What is the resultant site symmetry (remember to think in three dimensions)? Conjecture why it is not the same as what is listed. Use a diagram to help explain if necessary.

b. Briefly explain why one would not describe a crystal in which only the 1a site is occupied in this space group. What space group would be more correct?
3. Calculate the structure factor $F$ for the following reflections of an ideal cubic perovskite ($\text{ABO}_3$) in terms of $f_A$, $f_B$, $f_O$. Your answers should have no imaginary parts.

a) 100
b) 110
c) 111
d) 200

Which is likely to be the weakest of the four?

The atomic positions are:

A: 0 0 0
B: $\frac{1}{2} \frac{1}{2} \frac{1}{2}$
O: $\frac{1}{2} \frac{1}{2} 0$
$\frac{1}{2} 0 \frac{1}{2}$
0 $\frac{1}{2} \frac{1}{2}$
4. For the electron diffraction pattern shown below:

a. What are the indices of the reflection marked \( hkl \)?

b. What is the zone axis?

c. What can you conclude about the structure based on the systematic absences and the different spot intensities?
5. Briefly explain the Curie Principle.

6. An object with point symmetry $m\bar{3}m$ (O\textsubscript{h}) distorts under uniaxial stress along [001]. What is the point group of the distorted object? What is it when the stress is along [111]? If an applied electric field removes the centre of symmetry in each case, to which point groups would the distorted objects now belong?
7. Carbon atoms in graphite are bonded within (001) via strong triangular (120°) sp² hybrid σ bonding. The remaining unbonded 2p electrons form delocalized π bonds, and the adjacent sheets are held together by weak Van der Waals forces. For this reason, both the electrical and thermal conductivities of graphite are higher in the (001) than normal to it.

The thermal conductivity $k_{ij}$ is a tensor that relates the heat flux $h$ to the temperature gradient $dT/dx$ according to:

$$h_i = k_{ij} \frac{dT}{dx_j}$$

The thermal conductivity tensor of graphite is:

$$k_{ij} = \begin{bmatrix} 355 & 0 & 0 \\ 0 & 355 & 0 \\ 0 & 0 & 89 \end{bmatrix} \text{ Wm}^{-1}\text{K}^{-1}$$

a. If a gradient of 100 K/m is applied along the y direction, what is the resulting heat flow (in kW/m²)?

b. If a gradient of 100 K/m is applied along the z direction, what is the resulting heat flow (in kW/m²)?
8. The choice of unit cell is not unique and does not always reveal all of symmetry characteristics of a structure. Consider a hard-sphere model of a body-centred tetragonal structure with an arbitrary $c/a$ ratio ($c/a = \delta$). Assuming that spheres touch, three cases can be distinguished:

Case I: Spheres touch along $<001>$
Case II: Spheres touch along $<111>$
Case III: Spheres touch along $<100>$

(a) Calculate (by hand) the packing fraction as a function of $\delta$ for each case.
(b) Using Excel or another graphical software tool, plot the packing fraction as a function of $\delta$. Use linear axes with $0 \leq \delta \leq 3$ and $0 \leq PF \leq 1$ for your graph.
(c) Calculate (by hand) the values of $\delta$ at which realistic transitions from one case to another occur and indicate them on your graph? What is the Bravais lattice in each case? What is the Bravais lattice when $\delta = 1$? Illustrate your answers with Vesta or some other tool.
(d) Calculate (by hand) the packing fractions at these transitions and indicate them on your graph.
(e) Based on your calculations/graph above, what is the maximum packing fraction which occurs?