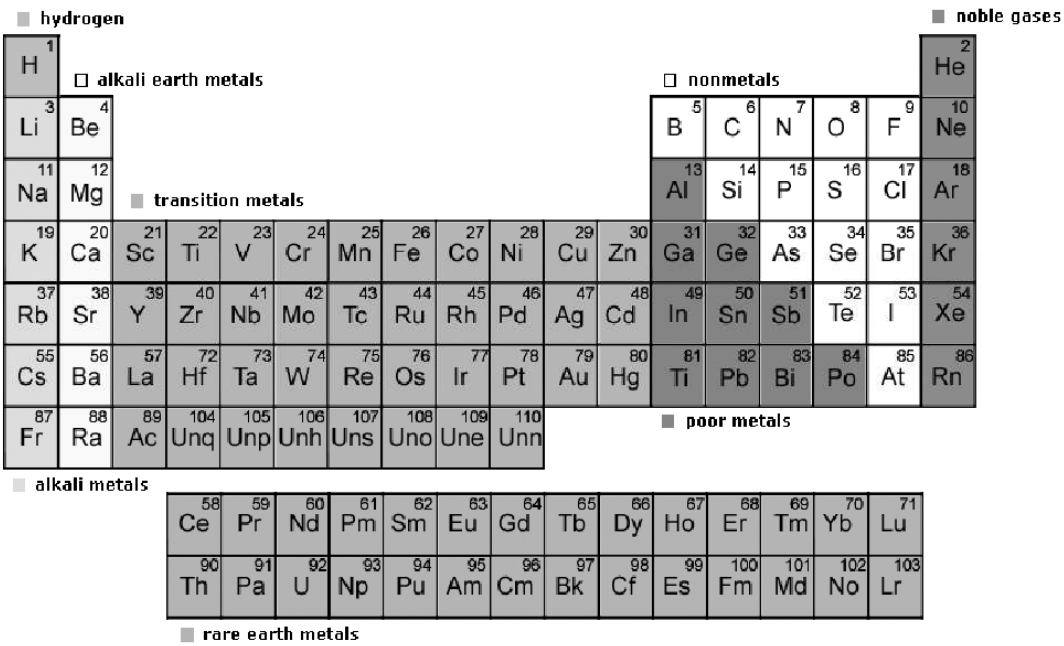
PHYSICS 315
Final examination: December 6, 2013

Answer all questions from all problems. Read all questions carefully. Where asked for a justification, a short one (a few words) will suffice. If you need extra booklets, ask me for them. Write your name and student number on each booklet, and turn all of them in. Talking to or looking at a neighbour's solution is not allowed, under any circumstances. All questions should be addressed to the invigilators. Attempts at academic misconduct will be severely penalized.

You may find some of the following equations useful:

- $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$.
- $S(\vec{G}) = \int_{\text{unit cell}} d\vec{r}\rho(\vec{r})e^{i\vec{G}\cdot\vec{r}}$.
- $e^{i\phi} = \cos(\phi) + i\sin(\phi)$.
- The Lennard-Jones potential is $U(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$.



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1. Consider a crystal made of Kr.

(a) What type of bonding is involved? Explain briefly its origin and what parameters are involved.

(b) Compare the simple cubic, the body-centered cubic and the face-centered cubic crystal structures. Which one is the actual structure? Hint: stop at the first row of neighbors when estimating cohesion energies.

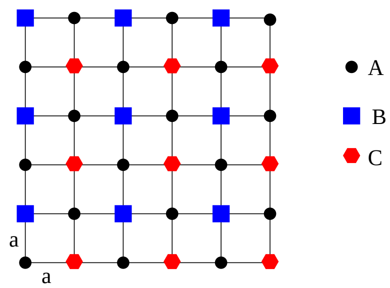
(c) What is the lattice constant of this material? Express the answer in terms of (some of) the parameters you listed at (a).

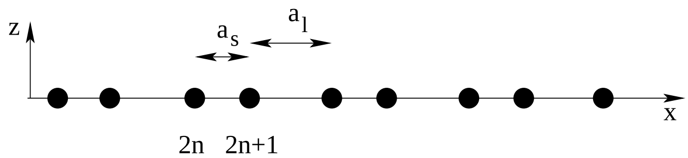
(d) Calculate the bulk modulus $B = -V\frac{\partial p}{\partial V}$, where the pressure is $p = -\frac{\partial U}{\partial V}$ and U is the energy of the crystal. Express the answer in terms of the parameters you listed at (a). Hint: express the volume in terms of the number of atoms (which is fixed) and the lattice constant (which changes with pressure).

2. Consider that $\rightarrow$ lattice, where A, B, and C are the elements with atomic numbers Z_A, Z_B and Z_c respectively. The length a is known.

(i) Find the location and intensity of all the Bragg peaks. Make a sketch showing the location and intensity of all these peaks.

(ii) what happens if all atoms are set to be identical, i.e. we take $Z_A = Z_B = Z_C = Z$?





3. Consider a one-dimensional chain made of identical atoms. The valence electrons occupy $2p_z$ orbitals, and there is one per atom. The distance between atoms alternates as shown in the figure above, with a_s, a_l being some known values.

(a) Assuming that $t_1 > t_2 > 0$, which of the following Hamiltonians properly describes nearest-neighbor hopping of the valence electrons in this system?

(i) $\mathcal{H} = -t_1 \sum_n (|2n\rangle\langle 2n+1| + |2n+1\rangle\langle 2n|) - t_2 \sum_n (|2n\rangle\langle 2n-1| + |2n-1\rangle\langle 2n|)$

(ii) $\mathcal{H} = -t_2 \sum_n (|2n\rangle\langle 2n+1| + |2n+1\rangle\langle 2n|) - t_1 \sum_n (|2n\rangle\langle 2n-1| + |2n-1\rangle\langle 2n|)$

(iii) $\mathcal{H} = t_1 \sum_n (|2n\rangle\langle 2n+1| + |2n+1\rangle\langle 2n|) + t_2 \sum_n (|2n\rangle\langle 2n-1| + |2n-1\rangle\langle 2n|)$

(iv) $\mathcal{H} = t_2 \sum_n (|2n\rangle\langle 2n+1| + |2n+1\rangle\langle 2n|) + t_1 \sum_n (|2n\rangle\langle 2n-1| + |2n-1\rangle\langle 2n|)$

(b) Find its eigenenergies and sketch them in the Brillouin zone.

(c) Is this a metal or an insulator?

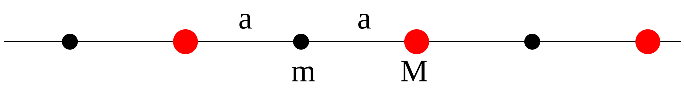
4. Answer briefly the following questions:

(i) Why do undoped (pure) semiconductors normally have a large resistivity?

(ii) Briefly explain why metals reflect light.

(iii) If you are told that a crystal has 2 longitudinal optical phonon modes, what information can you infer from this?

(iv) Consider the molecule C_2H_n. What values of n are possible? Sketch the shape of these molecules and briefly discuss what kinds of bonds keep the molecule stable for each possible value of n.



5. Consider the chain shown above, with atoms of mass m and M. In equilibrium, the distance between consecutive atoms is a, and there are a total of $2N$ atoms with periodic boundary conditions. We assume that only nearest-neighbour atoms interact, so that if they are at distance x their energy is $U(x) = \frac{K}{2}(x-a)^2$ where K is known. (i) Write Newton's second law for all these atoms, and find the corresponding frequencies of the normal modes. (ii) Sketch their energies in the Brillouin zone. Identify what types of phonons they are.