# Physics 406, Spring 2013

## Midterm I

## February 21, 2013

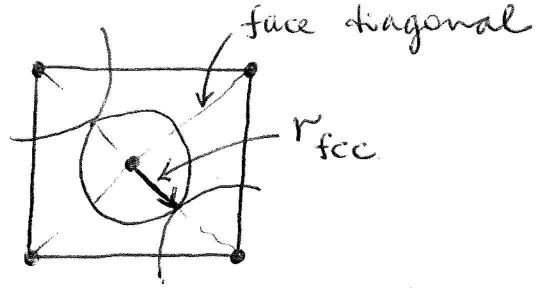
Name solutions

The five problems are worth 20 points each.

| Problem | Score |
|---|---|
| 1 | 20 |
| 2 | 20 |
| 3 | 20 |
| 4 | 20 |
| 5 | 20 |
| Total | 100 |

1. Find the packing ratios of 3D fcc and bcc lattices. Assume that all atoms are identical spheres. The packing ratio is defined as the maximum fraction of the unit cell volume taken up by the non-overlapping spheres.

fcc:



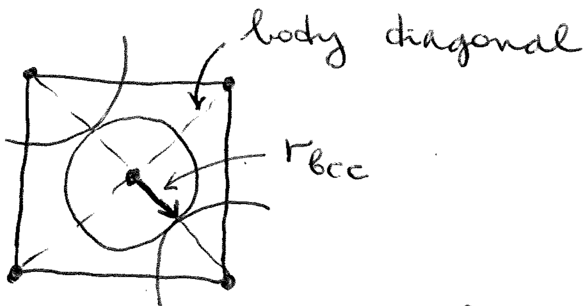

Spheres touch on the face diagonal:

$$r_{fcc} = \frac{a\sqrt{2}}{4}$$

Packing ratio $$P_f^{fcc} = \underset{\substack{\uparrow \\ \text{\# atoms per unit cell}}}{4} \times \left(\frac{4\pi}{3}\right)\left(\frac{a\sqrt{2}}{4}\right)^3 \frac{1}{a^3} =$$

$$= \frac{\pi\sqrt{2}}{6} \simeq 0.74.$$

bcc:




Spheres touch on the body diagonal:

$$r_{bcc} = \frac{a\sqrt{3}}{4}$$

$$P_f^{bcc} = \underset{\substack{\uparrow \\ \text{\# atoms per unit cell}}}{2} \times \left(\frac{4\pi}{3}\right)\left(\frac{a\sqrt{3}}{4}\right)^3 \frac{1}{a^3} = \frac{\pi\sqrt{3}}{8} \simeq 0.68.$$

Note that $P_f^{fcc} > P_f^{bcc}$.

2. Please answer the following conceptual questions:

a) Please describe why it is energetically favorable for valence electrons to delocalize (i.e. detach from their atoms) in metals.

Recall the uncertainty principle:

$$\Delta p \Delta x \sim \hbar$$

If $\Delta x \nearrow$ $\Delta p \searrow$, lowering the kinetic energy of the electron.

In metal, electrons delocalize over the entire sample & thus their energy is lowered.

b) Aluminum is less dense than uranium. Assuming that these two metals have roughly the same stiffness, what can you say about the expected speeds of sound in these two metals and why?

Recall that $v_s = \sqrt{\frac{Y}{\rho}}$.

Assuming that $Y_{Al} \simeq Y_u$,

$$\frac{v_s^{Al}}{v_s^{u}} = \sqrt{\frac{\rho_u}{\rho_{Al}}} > 1$$ , since $\rho_u > \rho_{Al}$.

Thus the speed of sound is greater in Al.

c) Vacancies are missing atoms in an otherwise near-perfect crystal. Since they create disorder and increase the entropy, vacancies are always present at non-zero temperatures in real crystals. How would you expect the X-ray diffraction of a crystal change due to a small number of vacancies?

We expect the X-ray diffraction pattern to be "washed out": the intensity of Bragg peaks will be reduced compared to an ideal crystal, and the intensity of background scattering will be somewhat increased.

d) Please describe main conceptual differences between Einstein and Debye theories of specific heat.

Einstein treated a solid as a collection of independent QM oscillators w/ frequency $\omega_E$.

Debye focused on sound waves propagating in a solid & caused by collective motions of atoms. The waves are treated as independent, and low-frequency, long-$\lambda$ modes are excited even at low Ts.

3. Please consider a monolayer of atoms that is a two-dimensional array in the (100) surface of the sc lattice. The cubic lattice constant is $a$ = 4 Å. Assume that the phonon dispersion is given by $\omega = ck$ .

a) What is the phonon density of states $D(\omega)$ for this 2D solid?

In 2D,

$$N(k) = \frac{\pi k^2}{\left(\frac{2\pi}{L}\right)^2}, \quad \text{where}$$

$L^2 = A$ is the area of the sample and $\pi k^2$ is the area of the circle w/radius k.

$$\text{So,} \quad N(k) = \frac{L^2 k^2}{4\pi}$$

$$\Downarrow \quad \omega = ck$$

$$N(\omega) = \frac{L^2 \omega^2}{4\pi c^2}$$

$$\Downarrow$$

$$D(\omega) = 2\frac{dN}{d\omega} = \underline{\underline{\frac{L^2 \omega}{\pi c^2}}}.$$

b) Assuming that the speed of sound in the monolayer is c = 3 x $10^3$ m/s, what is its Debye temperature? Note that
$\hbar = 1.05\times10^{-34} J\cdot s$, $k_B = 1.38\times10^{-23} J/K$.

Debye frequency is defined by

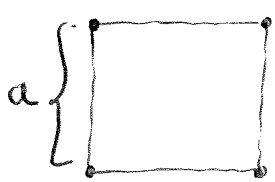
$$\int_0^{\omega_D} d\omega\, D(\omega) = \underset{\substack{\uparrow \\ 2D}}{2}N \text{ , or}$$

$$N(\omega_D) = N$$

$$\Downarrow$$

$$\frac{L^2\omega_D^2}{4\pi c^2} = N \text{ , or}$$

$$\omega_D = \Big[4\pi c^2 \underbrace{\left(\frac{N}{L^2}\right)}_{\text{2D atomic density}}\Big]^{1/2}$$




1 atom per 2D unit cell :

$$\frac{N}{L^2} = \frac{1}{16\ \text{Å}^2} .$$

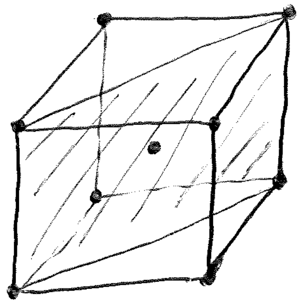
Then $\omega_D \simeq 2.66 \times 10^{13}\ 1/s$

Finally, $\theta_D \equiv \dfrac{\hbar\omega_D}{k_B} \simeq \underline{\underline{202.3\ K}}$

4. Please describe with a minimum of four sentences the key findings about disordered packing of ellipsoids reported in "Improving the Density of Jammed Disordered Packings Using Ellipsoids" by Donev et al. in Science (2004).

Key result: oblate spheroids pack more densely than do spheres when poured randomly and shaken. Experiments & computer simulations showed that random packing densities approach those of perfectly ordered arrangements of spheres. Used MRI to check that there was no periodic ordering in center. People always assumed that periodic orderings are denser than random ones => true for spheres but may not be true for spheroids. (!)

5. a) The Bragg angle for reflection from the (110) planes in bcc iron is 22 deg for an X-ray wavelength of $\lambda$ = 1.54 Å. Please find the cube edge for bcc iron (you can assume that n=1). What is the maximum wavelength with which the structure of this unit cell can be probed?




Bragg's law:

$$\lambda = 2d\sin\theta \qquad (n=1)$$

$$\Downarrow$$

$$d_{110} = \frac{\lambda}{2\sin\theta} = 2.06\ \text{Å}$$

Recall that $d_{hkl} = \dfrac{a}{\sqrt{h^2+k^2+l^2}}$ in a bcc lattice.

Then $a = d_{110}\sqrt{2} = 2.91\ \text{Å}$

The smallest distance between 2 atoms is $a$, so we need $\lambda < 2a$ for the scattering to be effective. Otherwise diffraction is impossible.

b) Using the result from (a), calculate the mass density of bcc iron. You can take the atomic weight of Fe to be 56.

$$\rho = \frac{\#\text{ Fe atoms}}{\text{Unit cell volume}} \times \frac{\text{Mol. weight of Fe}}{N(\#\text{ atoms per mole})} =$$

per unit cell

$$= \frac{2 \text{ atoms}}{(2.91 \times 10^{-8})^3 \text{ cm}^3} \times \frac{56 \text{ g/mole}}{6.02 \times 10^{23} \text{ atoms/mole}} \simeq$$

$$\simeq 7.58 \text{ g/cm}^3.$$