Physics 601

Midterm

October 23, 2015

Name Solutions

The five problems are worth 20 points each.

Problem	Score
1	
2	
3	
4	
5	
Total	

1. **Temperature-Dependence of the Bragg angle for Al.** At 300 K, Al has an fcc structure with a lattice constant of 0.405 nm. The coefficient of heat expansion for Al is $\alpha = 25 \times 10^{-6}\ K^{-1}$. Aluminum is studied with Cu $K_{\alpha 1}$ radiation which has a wavelength of $\lambda = 0.154$ nm. Let's now investigate the change $\Delta\theta$ in θ due to the change in temperature from 300 to 600 K.

(a) Derive the expression for $\Delta\theta$ in terms of θ. (10)

$$\frac{\Delta a}{a} = \alpha \Delta T = (25 \times 10^{-6}\ K^{-1})(300\ K)$$

$$= 7.5 \times 10^{-3}$$

$$\sin^2\theta = \frac{(h^2 + k^2 + l^2)\lambda^2}{4a^2}$$

$$2 \sin\theta \cos\theta\, d\theta = -\frac{\lambda^2}{2a^3}(h^2 + k^2 + l^2)\, da$$

$$= -\frac{2}{a} \sin^2\theta\, da$$

$$\Downarrow$$

$$d\theta = -(\tan\theta)\left(\frac{da}{a}\right)$$

$$\Delta\theta \approx -\tan\theta \left(\frac{\Delta a}{a}\right) = -\tan\theta\,(\alpha \Delta T)$$

$$\Delta\theta \approx -0.0075 \tan\theta$$ 2

(10).

(b) For the (111) reflection, evaluate $\Delta\theta$.

(111) reflection

$$\sin^2\theta_{111} = \frac{3\lambda^2}{4a^2} = \frac{3 \times (1.54)^2}{4 \times (4.05)^2} \approx .11$$

$$\sin\theta_{111} \approx 0.33$$

$$\tan\theta_{111} \approx 0.35$$

$$\Delta\theta \approx -0.15^\circ$$

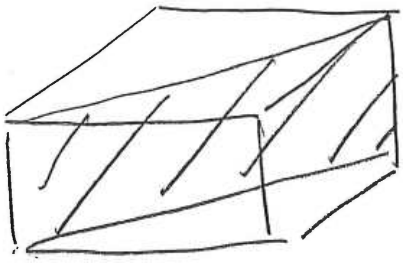
$$\Delta\theta \approx -.00261 \text{ radians.}$$

2 a) What is the n=1 Bragg angle for reflection from the (110) planes in bcc iron (cube edge = 2.91 Å) for an X-ray wavelength of λ = 1.54 Å? (10)

Bragg's Law (n=1)

$$\lambda = 2d \sin\theta$$

$$\sin\theta = \frac{\lambda}{2d}$$



bcc lattice

$$d = \frac{a}{\sqrt{h^2 + k^2 + l}}$$

$$d_{110} = \frac{a}{\sqrt{2}}$$

$$\sin\theta = \frac{\lambda}{2}\,\frac{\sqrt{2}}{a}$$

$$= \frac{(1.54)}{(2.91)}\,\frac{\sqrt{2}}{2} = .374$$

$$\Downarrow$$

$$\theta = 21.96^\circ \Rightarrow \theta \approx 22^\circ$$

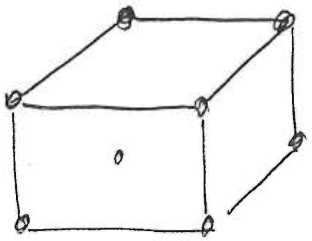
b) Please calculate the density of bcc iron. You can take the atomic weight of Fe to be 56 and Avogadro's number N = 6.02×10^{23} mol^{-1}. (10)

$$\rho = \frac{\#\ Fe\ atoms}{Volume\ of\ unit\ cell} \cdot \frac{Molecular\ weight\ of\ Fe\ (g\text{-}atom)}{N\ (\#\ atoms\ in\ 1\ g\text{-}mole)}$$

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

$$= \frac{(2)(56)}{(2.91)^3\ (6)}\ 10^{1}\ g/cm^3$$

bcc lattice



$$\frac{8\ corner\ atoms}{8\ cells}$$

$$\frac{1\ center\ atom}{1\ cell}$$

= 2 atoms / cell

$$\rho = 7.58\ g/cm^3$$

N.B. Textbook value

$\rho = 7.86\ g/cm^3$

for Fe !

3. Please consider a monolayer of element X that is a two-dimensional array of X atoms in the fcc (100) surface. The cubic lattice constant is 4 Å.

(5)

a) Let us suppose that the phonon dispersion for this layer has the form ck ($\omega \sim ck$). What is the phonon density of states $g(\omega)$ for this 2-d solid?

$$N(k) = \frac{\pi k^2}{\left(\frac{2\pi}{L}\right)^2} = \frac{A k^2}{4\pi}$$

$A = L^2$

$\omega = c.k \Rightarrow k = \left(\frac{\omega}{c}\right)$

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

$$g(\omega) = 2\,\frac{dN}{d\omega} = \frac{A\omega}{\pi c^2}.$$

2 modes / k-point (1 longitudinal, 1 transverse)

b) The speed of sound in bulk X is c = 5×10^3 m/s, and let's assume that this value is also appropriate for our monolayer. What is the Debye temperature for this X monolayer? (5)

You may need these constants

$\hbar = 1.05 \times 10^{-34}$ J-s

$k_B = 1.4 \times 10^{-23}$ J/K

$$k_B \Theta_D = \hbar \omega_D \Rightarrow \Theta_D = \frac{\hbar \omega_D}{k_B}$$

$$2N(\omega_D) = 2N \Rightarrow \omega_D$$

$$\frac{A \omega_D^2}{4\pi c^2} = 2N$$

X atoms = 2/cell = $\frac{2}{16 \text{ Å}^2}$

$$\Downarrow$$

$$\omega_D = \left\{ 4\pi c^2 \left(\frac{N}{A} \right) \right\}^{1/2}$$

$$= (4\pi)^{1/2} \; c \; \left(\frac{N}{A} \right)^{1/2}$$

$$= 2\sqrt{\pi} \left(5 \times 10^3 \right) \frac{1}{\sqrt{8} \times 10^{-10}}$$

$$= 4.7 \times 10^{13} \text{ s}^{-1}$$

$$\Theta_D = \frac{1.05 \times 10^{-34}}{1.4 \times 10^{-23}} \times 4.7 \times 10^{13}$$

$$\Theta_D = 3.53 \times 10^2 \text{ K}$$

$$\Theta_D = 353 \text{ K}$$

c) Using a Debye approach, please determine the temperature-dependence of the specific heat, $c_v(T)$, at low temperatures for this layer (you don't have to solve for all the coefficients and can leave them as definite integrals that are equal to constants). (5)

$$u(T) = \int_0^{\omega_D} \frac{\hbar\omega\, g(\omega)\, d\omega}{e^{\hbar\omega/kT} - 1} = \int_0^{\omega_D} \frac{\hbar\omega \left(\frac{A\omega}{\pi c^2}\right) d\omega}{e^{\hbar\omega/kT} - 1}$$

$$x = \frac{\hbar\omega}{kT} \qquad x_0 = \hbar\omega_D/kT$$

$$= \frac{\hbar A}{\pi c^2} \left(\frac{kT}{\hbar}\right)^3 \int_0^{x_0} \frac{x^2\, dx}{e^x - 1}$$

$$\lim_{T\to 0} \iff \lim_{x\to\infty}$$

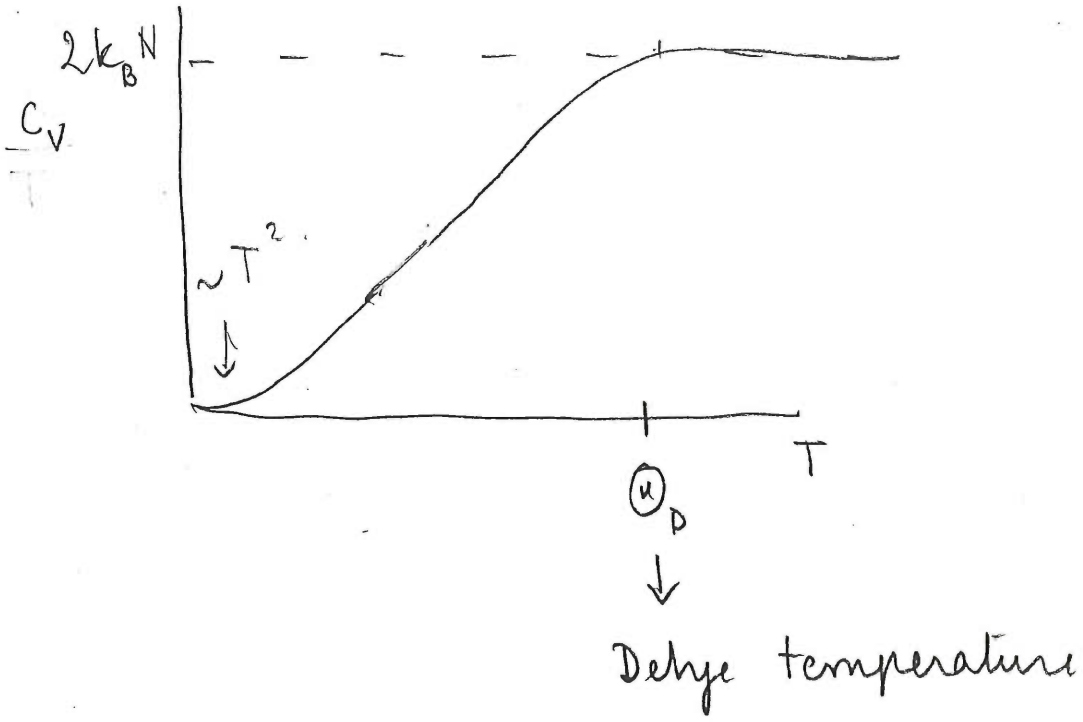
$$\lim_{T\to 0} u(T) = \frac{\hbar A}{\pi c^2} \left(\frac{kT}{\hbar}\right)^3 \underbrace{\int_0^{\infty} \frac{x^2\, dx}{e^x - 1}}$$

$X_0 = \text{constant}$

$$\lim_{T\to 0} c_V = \left(\frac{\partial u}{\partial T}\right)_V = \underbrace{[\quad]}_{\text{constant}} T^2$$

$$\boxed{\lim_{T\to 0} c_V \sim T^2}$$

d) Sketch the specific heat of the monolayer of X as a function of temperature, indicating important temperature scales. (5)



4. a) Using a free electron model, please derive an expression for the radius of the Fermi sphere in k-space as a function of n where n is the electron concentration. (6)

$$n = \frac{N}{V} = 2 \frac{1}{(2\pi)^3} \frac{4}{3} \pi k_F^3$$

$$\Downarrow$$

$$n = \frac{1}{3\pi^2} k_F^3 \Rightarrow \boxed{k_F = (3\pi^2 n)^{1/3}}$$

b) Monovalent Cu crystallizes in a fcc lattice with reciprocal lattice vectors

A = 2π/a (1, -1, 1)
B = 2π/a (1, 1, -1)
C = 2π/a (-1, 1, 1).

By determining the distance between the Fermi sphere and the Brillouin zone face, please give an argument, within the nearly free electron model, for why fcc Cu is expected to be a good metal.

$$k_i = \frac{1}{2} \frac{2\pi}{a} \left(1^2 + 1^2 + 1^2\right)^{1/2}$$

$$= \frac{\sqrt{3}\,\pi}{a} = 1.7 \frac{\pi}{a}$$

For fcc Cu $n = \frac{4}{a^3}$

$$k_F = \left(3\pi^2 \frac{4}{a^3}\right)^{1/3} = \left(\frac{12}{4\pi}\right)^{1/3} \frac{\pi}{a}$$

$$= 1.5 \frac{\pi}{a}$$

$k_F < k_i$

Fermi surface does not touch BZ faces ⇒ free electron picture OK ✓ metal.

c) Please repeat the same calculation for divalent Zn in a fcc lattice. Discuss the expected electrical behavior based on the nearly free electron model.

For fcc Zn

$$n = \frac{8}{a^3}$$

$$k_F = \left(3\pi^2 \frac{4}{a^3} \right)^{1/3} = \left(\frac{24}{\pi} \right)^{1/3} \frac{\pi}{a}$$

$$= 1.8 \; a$$

$k_F > k_i \Rightarrow$ Band gaps will probably occur.

Bands must be modified by potential.

Free electron model must be modified to describe system.

5. Please answer the following conceptual questions.

a. What additional information would you request to determine whether a diffraction pattern is due to the scattering of charged particles or by electromagnetic radiation? (4)

For diffraction to occur $\lambda \sim$ interatomic spacing ($\sim 2\,\text{Å}$).

EM radiation $E = hf = \frac{hc}{\lambda} \Rightarrow \lambda = \frac{hc}{E}$

For charged particles $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} \Rightarrow \lambda = \frac{h}{\sqrt{2mE}}$

(non-relativistic)

$\lambda(E)$ would distinguish these types of scattering

b. Vacancies are missing atoms in an otherwise near-perfect crystal. Since they create disorder and increase the entropy, vacancies are always present at nonzero temperatures. How would you expect the X-ray diffraction of a crystal to change due to presence of a small number of vacancies? (4)

We expect reduced intensity in the Bragg peaks (compared to those of a perfect crystal) and some contribution to background scattering.

c. What is the physical origin of the electronic gaps in the nearly free electron model? Please explain. (4)

Bragg reflection is the physical origin of the gaps in the electronic spectrum. The Bragg condition, $k = \pm \frac{1}{2} G$, means that there is Bragg reflection at the Brillouin zone boundaries. Thus, here there will be no travelling wave solutions and only standing waves – hence the energy gaps at the BZBs.

d. What are quasicrystals and why was their discovery so controversial? (4)

Quasicrystals are solids whose atoms are arranged in neither periodic nor random structure. Before their identification it was believed that sharp diffraction spots implied translational symmetry. However the diffraction patterns of quasicrystalline materials are sharp and display "forbidden symmetries" known to be incompatible w/ space-filling structures. They defied the conventional wisdom of diffraction and initially many thought that their Bragg characterization could be explained by twinning or (random) glassiness.

(4)

e. Please explain how "anti-Bragg" scattering is used to monitor surface growth in samples.

In the anti-Bragg condition, the source, the sample and the detector are set up so that there is destructive interference between parallel planes in the crystalline sample. In this situation, specular reflection from the surface can be monitored to give information about layer-by-layer growth.