Physics 601

Midterm

November 4, 2016

Name ____________________________

Solutions

The five problems are worth 20 points each.

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1. (20 points) The Bragg angles of a certain reflection from copper is 47.75° at 20°C but is 46.6° at 1000°C. What is the coefficient of linear thermal expansion \( \chi \) of copper in units of inverse Kelvin?

\[
\begin{align*}
L_0 &= \frac{n\lambda}{2\sin \theta_0} & \theta_0 &= 47.75° & T &= 20°C \\
L &= \frac{n\lambda}{2\sin \theta_T} & \theta_T &= 46.6° & T &= 1000°C \\
L > L_0 \Rightarrow \chi > 0
\end{align*}
\]

\[
\chi = \frac{1}{L} \left( \frac{L - L_0}{T - T_0} \right) \frac{1}{\Delta T}
\]

\[
\chi = \left( 1 - \frac{\sin \theta_T}{\sin \theta_0} \right) \frac{1}{\Delta T}
\]

\[
\chi = 1.88 \times 10^{-5} \text{ K}^{-1}
\]
2. (20 points) At 20°C Copper is an fcc lattice with a lattice constant of 3.597 Å and it is often studied with CuK$\alpha_2$ radiation which has a wavelength of $\lambda = 0.154$ nm. Assuming that it maintains this structure over the temperature range of interest (see Problem 1), for the (111) reflection, please evaluate $\Delta \theta$.

\[(111)\text{ reflection} \Rightarrow (h^2 + k^2 + l^2) = 3. \quad \sin^2 \theta = \frac{\lambda^2 (h^2 + k^2 + l^2)}{4a^2} \]

\[
\sin^2 \theta_{111} = \frac{3\lambda^2}{4a^2} = \frac{3 \times (1.54)^2}{4 \times (3.597)^2} \approx 0.09.
\]

\[\sin \theta_{111} \approx 0.3\]

\[
\frac{\Delta \theta}{\Delta T} = \Delta \theta = \frac{\Delta \theta}{\Delta T} \Rightarrow \text{ need to relate } \Delta \theta \text{ and } \Delta T
\]

\[
\sin \theta = \frac{C}{L}
\]

\[
\cos \theta = -\frac{C}{L^2} \quad \text{dL}
\]

\[
\Delta \theta = \frac{1}{\theta} \frac{d\theta}{d\theta} = -\frac{C}{L^2} \cos \theta \frac{d\theta}{d\theta} = -\cot \theta \frac{\Delta \theta}{\Delta T}
\]

\[
\downarrow
\]

\[
\Delta \theta_{111} = -\lambda \Delta T \tan \theta_{111}
\]

\[
\tan \theta_{111} \approx 0.3
\]

\[
\Delta \theta_{111} = -(1.88 \times 10^{-5}) (980) (0.3)
\]

\[
\Delta \theta = -0.00553 \text{ radians}
\]

\[
\Delta \theta = -0.317^\circ
\]
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 6 Å.

   a) (5 points) Let us suppose that the phonon dispersion for this layer has the form \( \omega = \alpha k^2 \). What is the phonon density of states \( g(\omega) \) for this 2-d solid?

\[
N(k) = \frac{\pi k^2}{(2\pi L)^2} = \frac{AK^2}{4\pi} \Rightarrow k = \left( \frac{\omega}{c} \right)
\]

\[
A = L^2
\]

\[
N(\omega) = \frac{Aw^4}{4\pi c^4}
\]

\[
g(\omega) = 2 \frac{dN}{dw} = \frac{2Aw^3}{\pi c^4}
\]

2 modes / k-point

(longitudinal and transverse)
b) (5 points) The speed of sound in bulk $X$ is $c = 3 \times 10^3 \text{ m/s}$, and let's assume that this value is also appropriate for our monolayer. What is the Debye temperature for this $X$ monolayer?

You may need these constants:

$$\hbar = 1.05 \times 10^{-34} \text{ J s}$$
$$k_B = 1.4 \times 10^{-23} \text{ J/K}.$$ 

$$k_B \Theta_D = \hbar \omega_D \implies \Theta_D = \frac{\hbar \omega_D}{k_B}.$$ 

$$g(w) = 2 \frac{dN}{dw} \implies \int_0^{\omega_D} dN = \frac{1}{2} \int_0^{\omega_D} g(w) \, dw.$$ 

$\omega_D$ defined by

$$\int_0^{\omega_D} g(w) \, dw = 2N$$

Thus

$$N(\omega_D) = N$$

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

$$= \left( \frac{4 \pi}{18} \right)^{1/4} \left( 3 \times 10^3 \right) \left( \frac{1}{18 \times 10^{-20}} \right)^{1/4}$$

$$= \left( \frac{4 \pi}{18} \right)^{1/4} \times 3 \times 10^8 \text{ s}^{-1}$$

$$= 2.74 \times 10^8 \text{ s}^{-1}$$

Atoms of $X$ =

$$2/\text{atom} = \frac{2}{36 \text{ A}^2}$$

$$\Theta_D = \frac{1.05 \times 10^{-34}}{1.4 \times 10^{-23}} \times 2.74 \times 10^8 = 2.055 \times 10^3 \text{ K}.$$
c) (5 points) Using a Debye approach, please determine the temperature-dependence of the specific heat, \( cv(T) \), 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).

\[
U(T) = \int_0^\infty \frac{k w g(w) \, dw}{e^{kw/\kappa T} - 1} = \int_0^\infty \frac{k w \left( \frac{2A w^3}{c^4 \pi} \right) \, dw}{e^{kw/\kappa T} - 1}
\]

Let \( x = \frac{kw}{\kappa T} \), \( x_0 = \frac{km}{\kappa T} \)

\[
U(T) = \frac{2kA}{\pi c^4} \left( \frac{kT}{\hbar} \right)^5 \int_0^\infty \frac{x^4 \, dx}{e^x - 1}
\]

\[
\lim_{T \to 0} \quad \lim_{x_0 \to \infty}
\]

\[
\lim_{T \to 0} \frac{U(T)}{U_0} = \frac{2kA}{\pi c^4} \left( \frac{kT}{\hbar} \right)^5 \int_0^\infty \frac{dx \cdot x^4}{e^x - 1}
\]

\[
\lim_{T \to 0} \frac{CV}{U_0} \sim T^4 \quad \text{constant}.
\]

\[
\lim_{T \to 0} CV \sim T^4
\]

\[
\lim_{T \to 0} CV \sim T^4
\]
d) (5 points) Sketch the specific heat of the monolayer of X as a function of temperature, indicating important temperature scales.
4. The sun has a mass of $2.0 \times 10^{30}$ kg and a radius of $7.0 \times 10^8$ m. Let's assume that it consists completely of ionized hydrogen at a temperature of $10^7$ K and that it is spherical. Let us determine the nature of the proton and the electron gases in it through the following steps (please see the end of this problem for some constants that you may find useful):

a) (5 points) Please derive an expression for the Fermi energy of a three-dimensional Fermi gas.

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

$$k_F = \left(3 \pi^2 n \right)^{1/3}$$

$$E_F = \frac{\hbar^2}{2m} k_F^2 = \frac{\hbar^2}{2m} \left(3 \pi^2 n \right)^{2/3}$$

b) (5 points) Please find the number density of free particles (protons or electrons) in the sun.

$$n = \frac{N}{V} = \frac{M_\odot}{m_\text{H}} \frac{1}{\frac{4}{3} \pi R_\odot^3}$$

$$= \frac{\left(2 \times 10^{30}\right)}{1.6736 \times 10^{-27}} \frac{1}{\frac{4}{3} \pi \left(7 \times 10^8\right)^3}$$

$$n = 8.31 \times 10^{29} \text{ particles/m}^3$$
c) (5 points) Please find the Fermi energies of the proton and the electron gases.

\[ E_F^p = \frac{h^2}{2m_p} \left( \frac{3\pi^2 n}{8} \right)^{2/3} = \frac{h^2}{2m_p} \left( \frac{3}{8\pi} m \right)^{2/3} = 1.8 \times 10^{-2} \text{ eV} \]

\[ = 2.86 \times 10^{-21} \text{ J} \]

\[ E_F^e = E_F^p \frac{m_p}{m_e} = 32.8 \text{ eV} \]

\[ = 5.2 \times 10^{-18} \text{ J} \]


d) (5 points) Compare these two energies with \( k_B T \) \( (k_B = 1.38 \times 10^{-23} \text{ J/K}) \) to determine whether each gas is degenerate \( (k_B T \ll E_F, \text{ so that few particles have energies over } E_F) \) or nondegenerate \( (k_B T \gg E_F, \text{ so that few particles have energies below } E_F \text{ and the gas behaves classically}) \). Please state clearly the situation in each of these two cases.

\[ kT = (1.38 \times 10^{-23} \text{ J/K}) \cdot 10^7 = 1.4 \times 10^{-16} \text{ J} \sim 10^3 \text{ eV} \]

\[ k_B T > E_F^p \quad \text{and} \quad k_B T > E_F^e \]

Both gases are nondegenerate.

Here are some constants that you may find useful:

\[ h = 6.63 \times 10^{-34} \text{ J-s} \]
\[ m_H = 1.6736 \times 10^{-27} \text{ kg} \]
\[ m_P = 1.6726 \times 10^{-27} \text{ kg} \]
\[ m_E = 9.11 \times 10^{-31} \text{ kg} \]
\[ 1 \text{ eV} = 1.6 \times 10^{-19} \text{ J} \]
5. Please answer the following conceptual questions.

a. (5 points) What additional information would you request to determine whether a diffraction pattern is due to the scattering of charged particles or by electromagnetic radiation?

\[ \lambda \sim \text{interatomic spacing} \quad (\sim 2 \text{ Å}) \]

\[ \text{EM radiation} \quad E = hf = \frac{hc}{\lambda} \quad \Rightarrow \quad \lambda = \frac{hc}{E} \]

\[ \text{For charged particles} \quad \lambda = \frac{\hbar}{p} = \frac{\hbar}{\sqrt{2meE}} \quad \Rightarrow \quad \lambda = \frac{\hbar}{\sqrt{2meE}} \]

\text{(non-relativistic)}

\( \lambda(E) \) would distinguish these 2 types of scattering.

b. (5 points) 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?

We expect reduced intensity in the Bragg peaks (compared to those of a perfect crystal) and some contribution to background scattering.
c. (5 points) What are quasicrystals and why was their discovery so controversial?

Quasicrystals are solids whose atoms are arranged in neither periodic nor random structures. 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 with space-filling structures. They defied the conventional wisdom of diffraction and initially many thought that their Bragg characterization could be explained by twinning.

d. (5 points) 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.