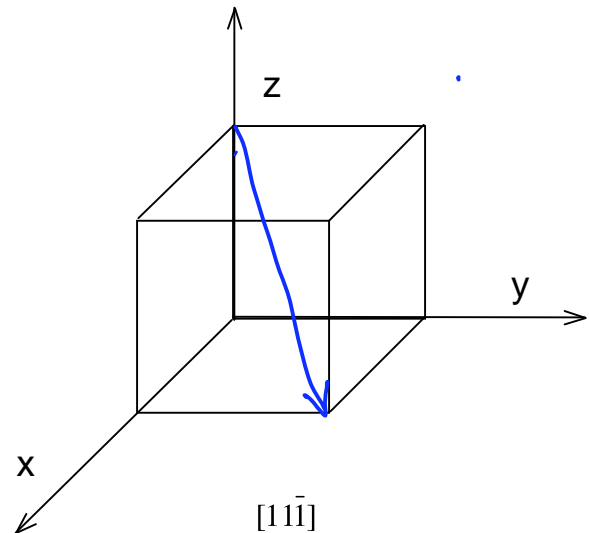
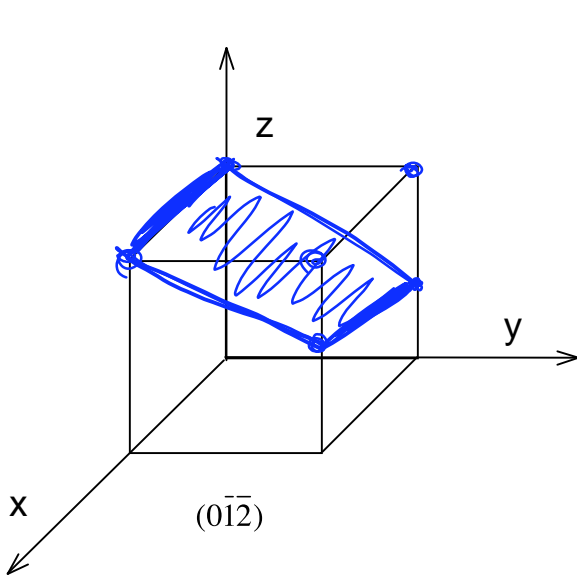


Problem #1 (22%)



(a) For each unit cell above, draw the crystallographic feature indicated and label it clearly. (8%)

(b) Named after Salvadore Dali, dalium (Da) is BCC. Its molar volume is $6.66 \text{ cm}^3/\text{mol}$. Calculate the density of atoms in (001) of Da. Express your answer in atoms/cm².

(8%)

BCC

$$\frac{Z}{a^3} = \frac{N_A V}{V_m} \therefore a = \left(\frac{2 V_m}{N_A} \right)^{1/3}$$

$$= 2.81 \times 10^{-8} \text{ cm}$$

$\therefore \frac{1}{(2.81 \times 10^{-8})^2} = 1.27 \times 10^{15} / \text{cm}^2$

(c) Here is the (011) plane in a unit cell of magnesium oxide (MgO) which is FCC. Indicate the positions of all atoms lying in the plane. Represent atoms as 2-dimensional slices of space-filling spheres. The values of ionic radii are $\text{Mg}^{2+} = 0.65 \text{ \AA}$ and $\text{O}^{2-} = 1.34 \text{ \AA}$. Your sketch need not be drawn to scale; however, you must convey relative values of the ionic dimensions.

(6%)

• lattice point

○ O^{2-}

● Mg^{2+}

Problem #2 (23%)

- (a) You discover that someone has been using your x-ray generator and has changed the target/anode. To determine the chemical identity of the new target, you go ahead and operate the x-ray generator and find the wavelength, λ , of the K_α peak to be 0.250 nm. What element is the target made of?

(7%)
$$\bar{V}_{K_\alpha} = \frac{3}{4} R (Z-1)^2 = \frac{1}{\lambda} \Rightarrow Z = 1 + \left(\frac{4}{3\lambda R} \right)^{1/2}$$

$$\therefore Z = 1 + \left(\frac{4}{3 \times 2.50 \times 10^{-10} \times 1.1 \times 10^7} \right)^{1/2} = 23$$

$$\therefore \text{The element is V (Vanadium)}$$

- (b) Hilary Sheldon conducts an experiment with her x-ray diffractometer. A specimen of tantalum (Ta) is exposed to a beam of monochromatic x-rays of wavelength set by the K_α line of titanium (Ti). Calculate the value of the smallest Bragg angle, θ_{hkl} , at which Hilary can expect to observe reflections from the Ta specimen.

DATA: λ_{K_α} of Ti = 2.75 Å; lattice constant of Ta, $a = 3.31$ Å

(9%)
$$\lambda = 2d \sin \theta \quad \therefore \text{Smallest } \theta \text{ is associated with the largest } d \text{ spacing}$$

Ta is BCC $\therefore h+k+l$ even \therefore largest (hkl) is $(011) \Rightarrow \theta = \sin^{-1} \left(\frac{\lambda}{2d} \right)$ where $d = \frac{a}{(h^2+k^2+l^2)^{1/2}}$

$$= \sin^{-1} \left(\frac{2.75}{2 \times \frac{3.31}{\sqrt{2}}} \right) \quad \parallel \quad = \frac{3.31}{(0+1+1)^{1/2}}$$

$$= 36^\circ \quad \parallel \quad = 3.31/\sqrt{2}$$

- (c) Sketch the emission spectrum (intensity versus wavelength) of an x-ray target that has been bombarded with **photons** instead of with electrons. Assume that the incident photons have more than enough energy to dislodge K-shell electrons in the target. On your spectrum label the features associated with K_α radiation, K_β radiation, and L_α radiation.

(7%) with photons, expect to see characteristic lines but NO BREMSSTRAHLUNG \therefore interaction between photons & atoms of target causes no photon deflection



Problem #3 (28%)

- (a) Germanium (Ge) is a semiconductor with a band gap energy, E_g , of 0.7 eV. Determine the amount (in grams) of gallium (Ga) that substitutionally incorporated into 1 kg of Ge will establish a charge-carrier concentration of 3.091×10^{17} carriers/cm³. You may assume that the temperature is sufficiently high that all of the doping states are fully ionized.

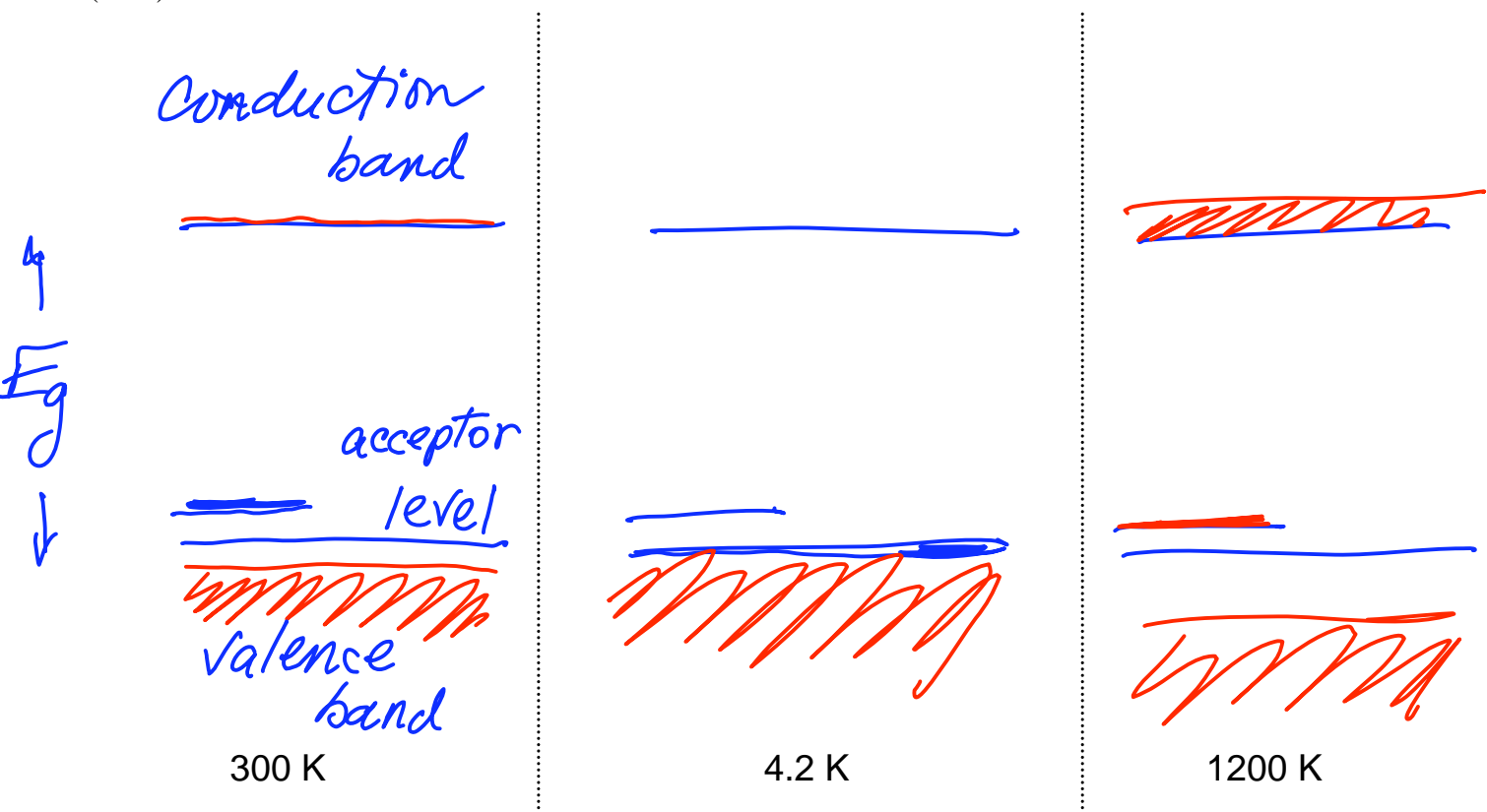
(11%) *1 carrier / Ga dopant atom*
 \therefore we need 3.091×10^{17} Ga atoms/cm³ Ge
 $\Rightarrow (3.091 \times 10^{17} / N_{Av} \text{ moles Ga}) \times 69.723 \frac{\text{g}}{\text{mole}} = 3.58 \times 10^{-5} \frac{\text{g Ga}}{\text{cm}^3 \text{ Ge}}$
 Volume of 1 kg Ge = $\frac{1000 \text{ g}}{5.35 \text{ g/cm}^3} = 187 \text{ cm}^3$
 \therefore mass of Ga dopant req'd = $3.58 \times 10^{-5} \times 187 = \underline{\underline{6.69 \times 10^{-3} \text{ g}}}$

- (b) Name the dominant charge carrier in Ga-doped Ge, and specify whether the material is p- or n-type.

(4%) h^+ (hole) \therefore p-type

- (c) Draw the schematic energy-level diagram of Ga-doped germanium indicating electron occupancy at ① 300 K (room temperature); ② 4.2 K (cooled in liquid helium); ③ 1200 K (heated to near the melting point of Ge). Label the (1) valence band, (2) conduction band, (3) energy gap, and (4) any energy levels associated with the presence of the dopant. Show electron occupancy by shading.

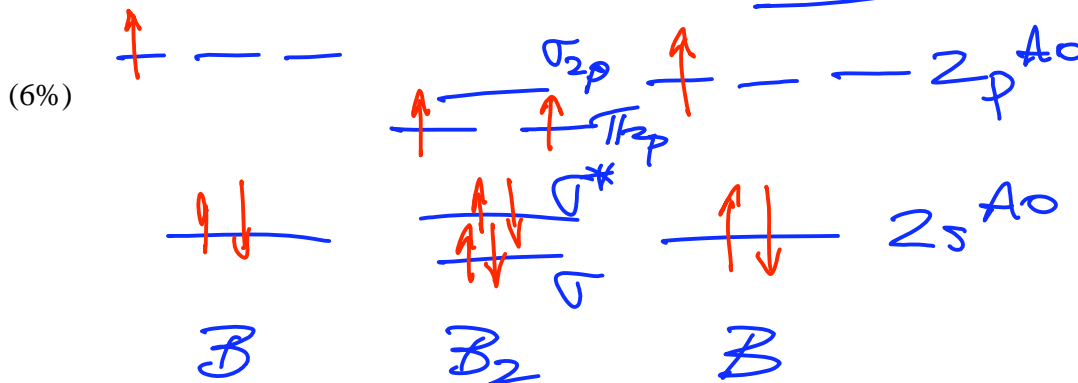
(13%)



Problem #4 (16%)

- (a) Boron exists in the gas state as the dimer, B_2 . Explain how the fact that B_2 is paramagnetic (two unpaired electrons) implies that in this molecule the π_{2p} orbitals must lie at a lower energy than do

B is $2s^2 2p^1$ // only if $\pi_{2p} < \sigma_{2p}$ will the two $2p$ electrons be unpaired \Rightarrow



from diagram you can see that if $\sigma_{2p} < \pi_{2p}$ both electrons would occupy $\sigma_{2p} \Rightarrow$ paired

- (b) Is the gas molecule, B_2^{2-} , more or less stable than the gas molecule, B_2 ? Explain.

- B_2^{2-} has two more electrons than B_2
- these two electrons pair up with the two unpaired electrons in the π_{2p} orbitals, thereby forming two bonds
- hence, we expect B_2^{2-} to be **more stable** than B_2

(4%)

- (c) Aluminum arsenide (AlAs) is a compound semiconductor with a band gap energy, E_g , of 2.3 eV. The value of E_g can be decreased by mixing AlAs with a compound semiconductor that has a smaller band gap energy. Name one such compound semiconductor and justify your choice by making reference to the operative chemical bonding.

(6%) Smaller $E_g \Rightarrow$ weaker bond
 \Rightarrow greater internuclear sepⁿ

\therefore choose group 13 below Al: Ga, In
 group 15 below As: Sb

\Rightarrow GaAs, InAs, AlSb

Problem #5 (11%)

- (a) Which compound do you expect to have the **higher** boiling point: HF or NH₃? Justify your choice with an explanation, using narrative or cartoons or both, that makes reference to the operative chemical bonding.

(6%) Compare $\Delta\chi$ within HF & NH₃
 \Rightarrow HF bond is more polar
 also F has 3 nonbonding electron pairs
 \therefore HF capable of stronger H-bonding
 \Rightarrow expect HF to have higher b.p.

- (b) To which does an atom of Ar form a stronger bond: another Ar atom or an atom of Kr? Justify your choice with an explanation, using narrative or cartoons or both, that makes reference to the operative chemical bonding.

- operative bonding in both cases is van der Waals
 (5%) - Compare $\text{Ar} \text{Ar}$ to $\text{Ar} \text{Kr}$
 Kr has more electrons & is larger than Ar
 $\therefore \alpha$ (polarizability) of Kr $>$ α (Ar)
 \therefore Ar-Kr bond is stronger