3.091 OCW Scholar

Self-Assessment Exam
Crystalline Materials

Solution Key

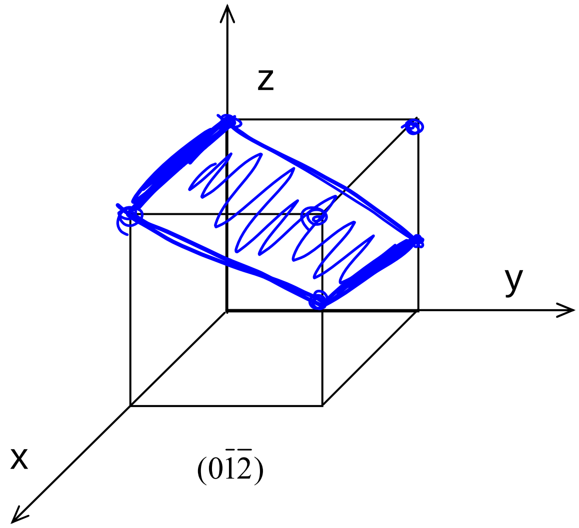
Write your answers on these pages.

State your assumptions and show calculations that support your conclusions.

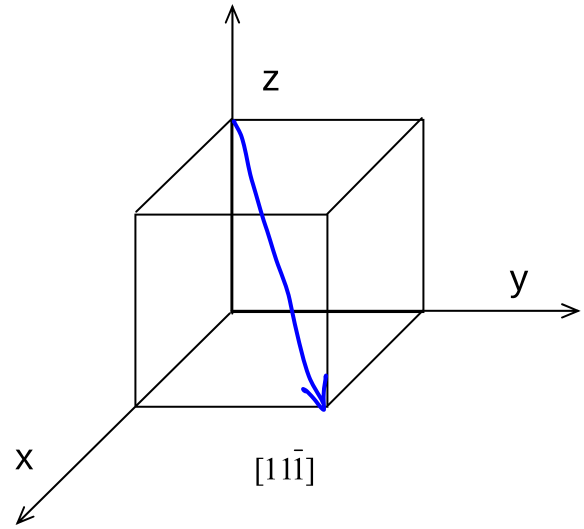
RESOURCES PERMITTED: PERIODIC TABLE OF THE ELEMENTS, TABLE OF CONSTANTS, AN AID SHEET (ONE PAGE 8½" × 11"), AND A CALCULATOR.

NO BOOKS OR OTHER NOTES ALLOWED.

Exam 2, Problem #1



$(0\bar{1}\bar{2})$



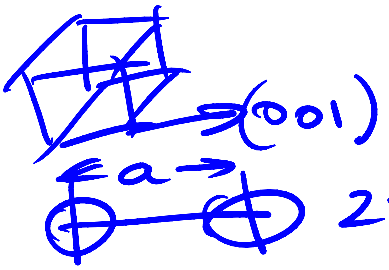
$[11\bar{1}]$

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

(b) Named after Salvadore Dali, dalium (Da) is BCC. Its molar volume is 6.66 cm^3/mol. Calculate the density of atoms in (001) of Da. Express your answer in atoms/cm^2.

BCC

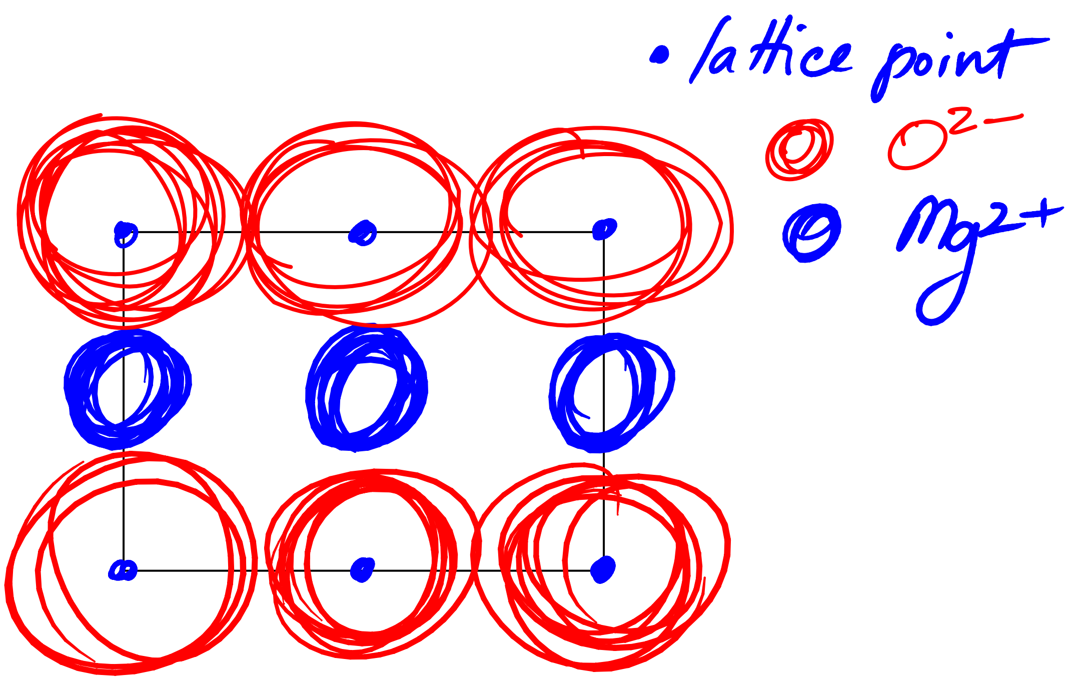
$$\frac{2}{a^3} = \frac{N_{Av}}{V_m} \quad \therefore \; a = \left(\frac{2V_m}{N_{Av}}\right)^{1/3} = 2.81\times10^{-8}\ cm$$



$2\times\frac{1}{2} = 1$ atom/a

$$\therefore \frac{1}{(2.81\times10^{-8})^2} = 1.27\times10^{15}/cm^2$$

(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 Mg^{2+} = 0.65 Å and O^{2-} = 1.34 Å. Your sketch need not be drawn to scale; however, you must convey relative values of the ionic dimensions.



Exam 2, Problem #2

(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 Å. What element is the target made of?

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

$$\therefore Z = 1 + \left(\frac{4}{3 \times 2.50\times10^{-11} \times 1.1\times10^{7}}\right)^{1/2} = 23$$

∴ 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

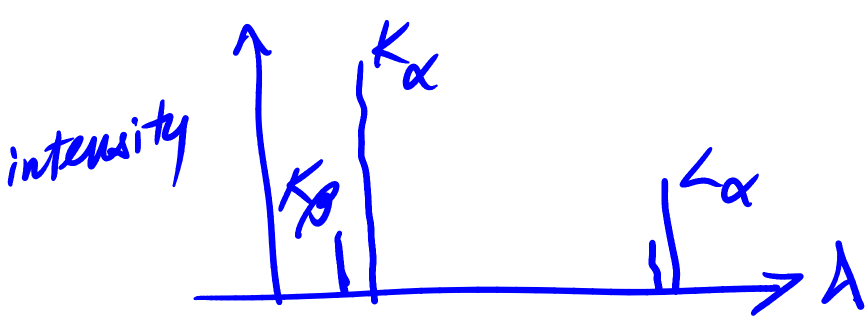
$\lambda = 2d\sin\theta$ ∴ smallest θ is associated with the largest d spacing

Ta is BCC ∴ h+k+l even ∴ largest (hkl) is (011) $\Rightarrow \theta = \sin^{-1}\left(\frac{\lambda}{2d}\right)$ where $d = \frac{a}{(h^2+k^2+l^2)^{1/2}} = \frac{3.31}{(0+1+1)^{1/2}} = 3.31/\sqrt{2}$

$$= \sin^{-1}\left(\frac{2.75}{2 \times \frac{3.31}{\sqrt{2}}}\right) = 36^\circ$$

(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.

With photons, we expect to see the characteristic lines but NO Bremsstrahlung, because the interaction between photons and atoms in the target causes no deflection.



Exam 3, Problem #1

Silver bromide (AgBr) has rock salt crystal structure, i.e., FCC Bravais lattice with the ion pair, Ag^+ and Br^- as basis. The dominant defect in AgBr is the Frenkel disorder.

(a) Does the Frenkel disorder in AgBr create vacancies of Ag^+, vacancies of Br^-, or both? Explain. The ionic radii are 0.67 Å for Ag^+ and 1.96 Å for Br^-.

We expect the smaller ion to form interstitials and create vacancies. Here, Ag^+ is the smaller ion, so there should be Ag^+ interstitials and vacancies on the Ag^+ sublattice.

(b) Calculate the temperature at which the fraction of Frenkel defects in a crystal of AgBr exceeds 1 part per billion = 1 ppb = 10^{-9}. The enthalpy of Frenkel defect formation, ΔH_F, has a value of 1.16 eV / defect, and the entropic prefactor, A, has a value of 3.091.

$$f_v = A \exp -\frac{\Delta H_F}{k_B T} \Rightarrow \ln f_v = \ln A - \frac{\Delta H_F}{k_B T} \Rightarrow \frac{\Delta H_F}{k_B T} = \ln A - \ln f_v$$

$$\therefore \quad T = \left\{ \frac{k_B}{\Delta H_F} \left(\ln A - \ln f_v \right) \right\}^{-1}$$

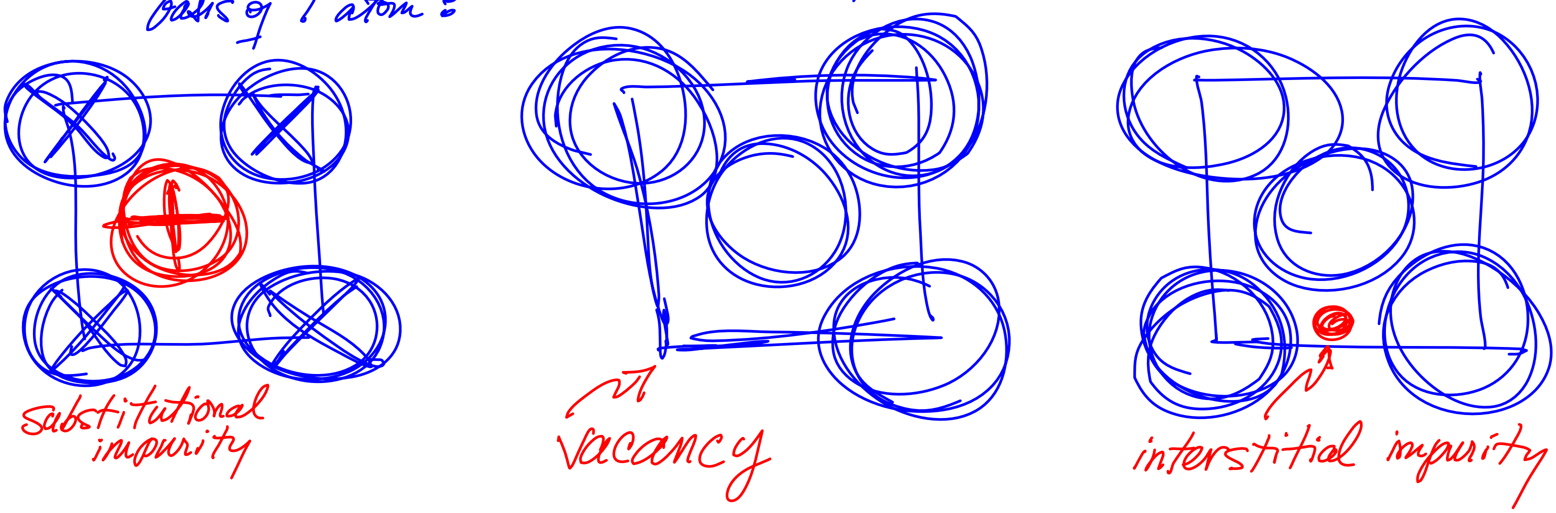
$$= \left(\frac{10^{-23}}{1.16 \times 1.6\times 10^{-19}} \left(\ln 3.091 - \ln 10^{-9} \right) \right)^{-1} = 615\ K = 342°C$$

↑ converting eV to J

Exam 3, Problem #2

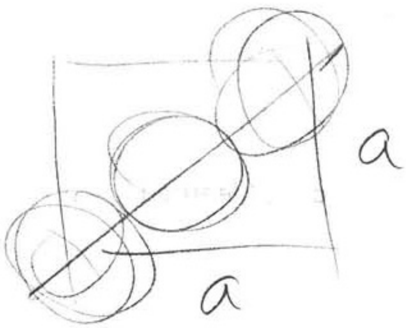
(b) On each of three separate drawings of one face of an FCC unit cell, indicate one of each of the following: (1) substitutional impurity; (2) vacancy; (3) interstitial impurity.

assume close-packed hard-sphere model of atomic packing & basis of 1 atom:



Final Exam, Problem #3

(b) Calculate the atomic packing density along [011] direction of aluminum (Al). Express your answer in units of atoms cm^{-1}.



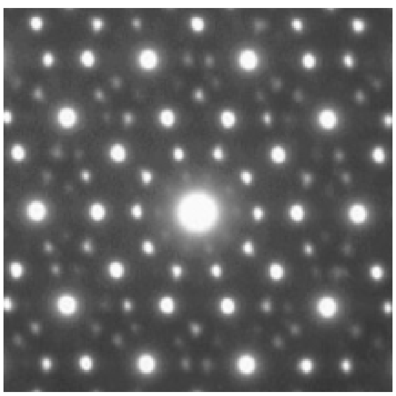
$$\frac{2}{\sqrt{2}\,a}$$

$$\frac{4}{a^3} = \frac{N_{Av}}{V_{molar}}$$

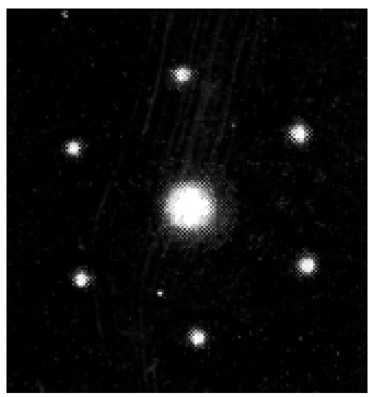
$$\therefore a = \left(\frac{4V_m}{N_{Av}}\right)^{1/3}$$

Final Exam, Problem #4

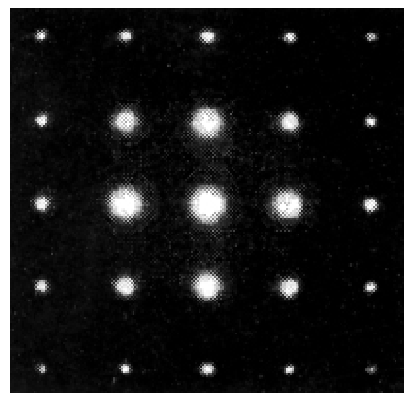
Give the rotational symmetry of each of the following patterns. Express your answer as *n*-fold.



5-fold



3-fold



4-fold