EMA 5104 Homework #1
Due Monday, September 14th at 9am

1. Give the electron configurations for Al^{3+} and O^{2-}.

Al^{3+}: From Table 2.2, the electron configuration for an atom of aluminum is $1s^2 2s^2 2p^6 3s^2 3p^1$. To become an ion with a plus three charge, it must lose three electrons—two 3*s* and the one 3*p*. Thus, the electron configuration for an Al^{3+} ion is $1s^2 2s^2 2p^6$.

O^{2-}: From Table 2.2, the electron configuration for an atom of oxygen is $1s^2 2s^2 2p^4$. To become an ion with a minus two charge, it must acquire two electrons—in this case another two 2*p*. Thus, the electron configuration for an O^{2-} ion is $1s^2 2s^2 2p^6$.

2. Compute the percentage ionic character of the interatomic bond for each of the following compounds: MgO, GaP, CsF, CdS, and FeO.

$$\%IC = \{1 - \exp[-(0.25)(X_A - X_B)^2]\} \times 100$$

MgO: $X_{Mg} = 1.3, X_O = 3.5$, $\%IC = \{1 - \exp[-(0.25)(3.5 - 1.3)^2]\} \times 100 = 70.2\%$

GaP: $X_{Ga} = 1.8, X_P = 2.1$, $\%IC = \{1 - \exp[-(0.25)(2.1 - 1.8)^2]\} \times 100 = 2.2\%$

CsF: $X_{Cs} = 0.9, X_F = 4.1$, $\%IC = \{1 - \exp[-(0.25)(4.1 - 0.9)^2]\} \times 100 = 92.3\%$

CdS, $X_{Cd} = 1.5, X_S = 2.4$, $\%IC = \{1 - \exp[-(0.25)(2.4 - 1.5)^2]\} \times 100 = 18.3\%$

FeO, $X_{Fe} = 1.7, X_O = 3.5$, $\%IC = \{1 - \exp[-(0.25)(3.5 - 1.7)^2]\} \times 100 = 55.5\%$

3. The interatomic potential energy, U, is given by the following equation.

$$U = -\frac{A}{r} + \frac{B}{r^{10}}$$

Given that the atoms form a stable molecule at a separation of 0.35 nm with an energy of - 6.13 eV.

a) Calculate A and B
b) Find the force required to break the bond (max force, F_{max}) and the corresponding critical separation.
c) Find the Young's modulus (E) in GPa.

(a)

$$U = -\frac{A}{r} + \frac{B}{r^{10}}$$

$$1\ eV = 1.60218\ x\ 10^{-19}\ J$$

At a stable separation under equilibrium, $\frac{dU}{dr}|_{r=r_0} = \frac{A}{r_0^2} - \frac{10B}{r_0^{11}} = 0$

$$r_0^9 = \frac{10B}{A} \qquad \cdots\cdots (1)$$

From a given condition of U = -6.13eV at r_0 = 0.35 nm

$$U = -\frac{A}{r} + \frac{B}{r^{10}}$$

$$Ur_0^{10} = -Ar_0^9 + B \qquad \cdots\cdots (2)$$

From (1) and (2), $Ur_0^{10} = -9B$

$$B = -\frac{U{r_0}^{10}}{9} = \frac{6.13 \times (0.35)^{10}}{9} = 1.88 \times 10^{-5} eV \cdot nm^{10} = 3.0 \times 10^{-24} J \cdot nm^{10}$$

$$A = \frac{10B}{r_0^9} = 2.39 eV \cdot nm = 3.8x10^{-19} J \cdot nm$$

(b) Maximum force (force required to break) is obtained by (note: this is not the force at r=r_0)

$$\frac{d^2U}{dr^2} = -\frac{2A}{r^3} + \frac{110B}{r^{12}} = 0$$

$$r = \left(\frac{110B}{2A}\right)^{1/9} = 0.423nm$$

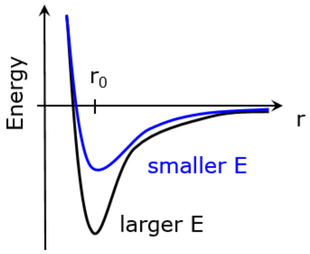
$$F = \frac{dU}{dr}|_{r=0..423nm} = \frac{A}{r^2} - \frac{10B}{r^{11}} = \frac{10.93\text{eV}}{nm} = 1.75 \times 10^{-18} J/n\,m = 1.75 \times 10^{-9} N$$

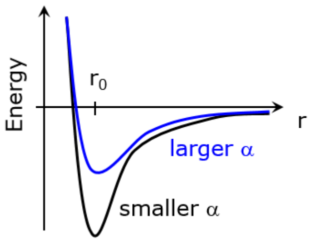
(c)

$$E = \frac{1}{r_0}\left(\frac{d^2U}{dr^2}\right)_{r=0.35nm} = \frac{1}{r_0}\left(-\frac{2A}{{r_0}^3} + \frac{110B}{{r_0}^{12}}\right) = 2.286 \times 10^{-16} J/n\,m^3 = 228.6\ GPa$$

4. Explain why it is difficult to find a material with both a high stiffness and a high coefficient of thermal expansion.

The elastic modulus is proportional to the curvature of the bonding energy at r_0. $E \propto \frac{\partial^2 U}{\partial r^2}|r_0$. The modulus is larger for deeper potential wells. CTE has to do with the asymmetry of the potential well. Deeper potential wells appear more symmetric. So CTE decreases as the well depth increases.





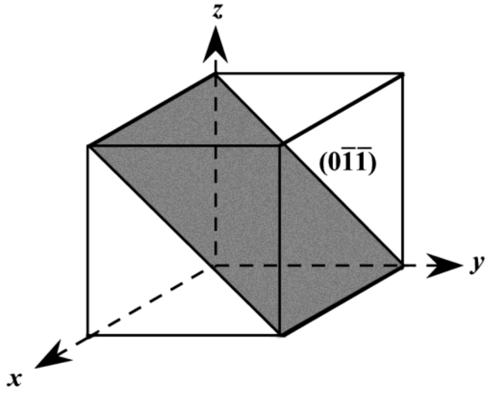
5. Niobium (Nb) has a BCC crystal structure, an atomic radius of 0.143 nm and an atomic weight of 92.91 g/mol. Calculate the theoretical density for Nb.

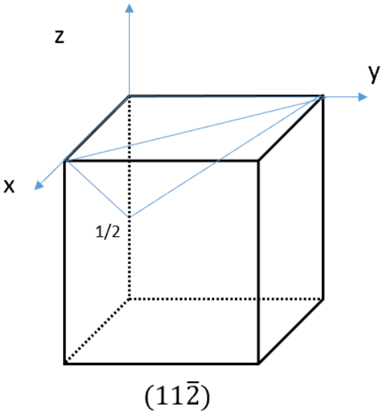
$\rho = \frac{nA_{Nb}}{V_C N_A}$, n = 2 atoms/unit cell for BCC. $V_C = a^3$, $a = \frac{4R}{\sqrt{3}}$, therefore $V_C = \left(\frac{4R}{\sqrt{3}}\right)^3$

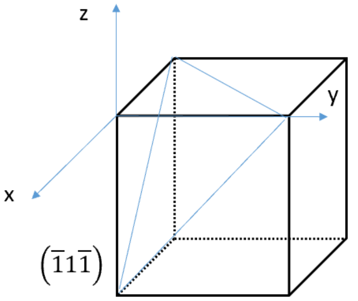
A_{Nb} = 92.91 g/mol, $\rho = \frac{nA_{Nb}}{\left(\frac{4R}{\sqrt{3}}\right)^3 N_A}$=8.48 g/cm^3

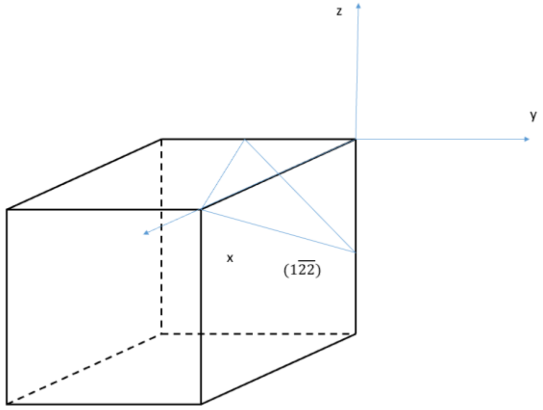
Note the experimental density for Nb is 8.57 g/cm^3.

6. Draw the following planes for a cubic structure. $(0\bar{1}\bar{1}), (11\bar{2}), (\bar{1}1\bar{1}), (1\bar{2}\bar{2})$

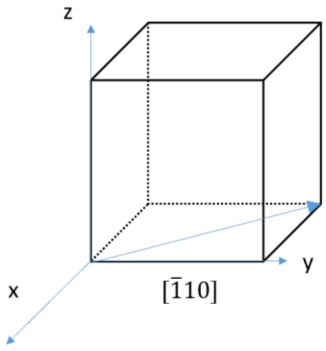


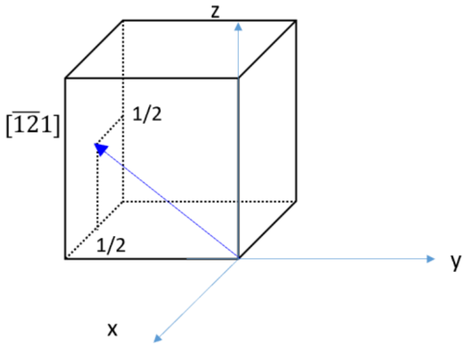


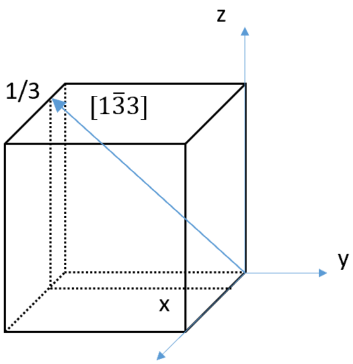


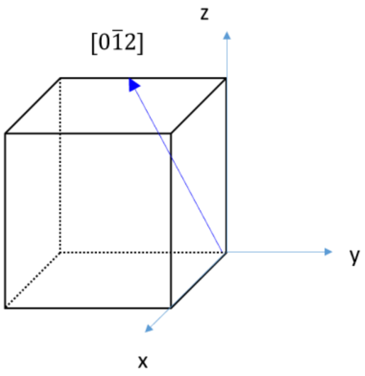


7. Draw the following directions for a cubic structure. $[\bar{1}10], [\bar{1}21], [1\bar{3}3], [0\bar{1}2]$

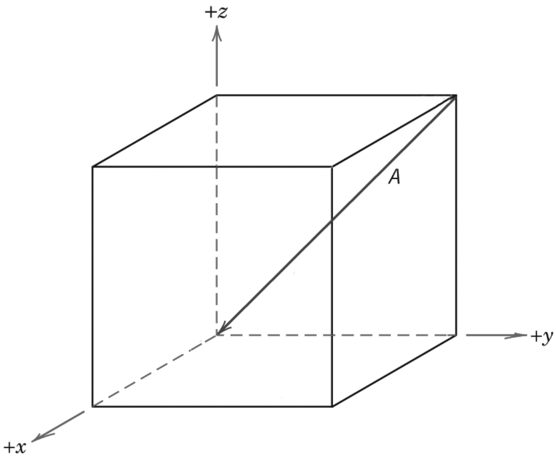

z
y
x
$[\bar{1}10]$

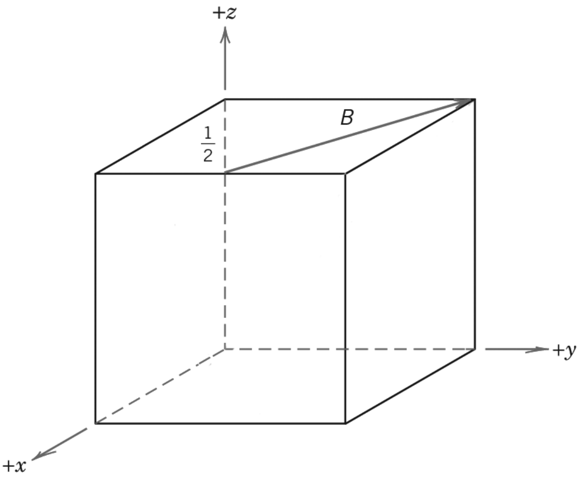

z
$[\bar{1}\bar{2}1]$
1/2
1/2
y
x

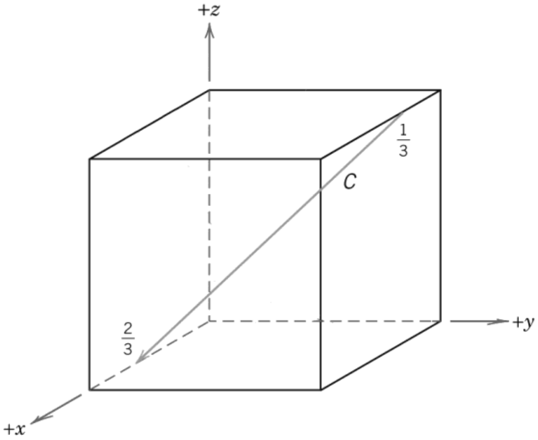

z
1/3
$[1\bar{3}3]$
y
x

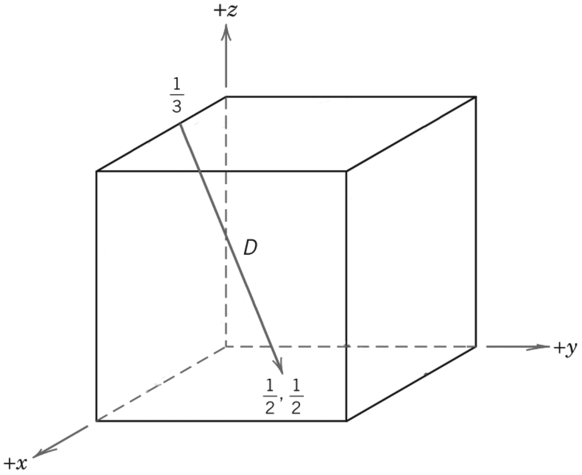

z
$[0\bar{1}2]$
y
x

8. Determine the Miller indices for the directions shown in the following cubic unit cell









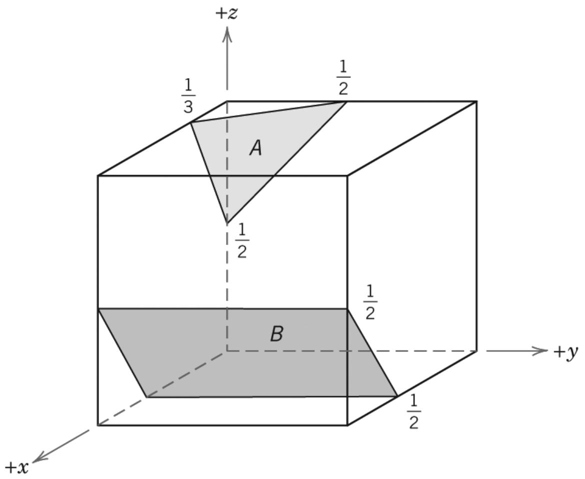
A: $[0\bar{1}\bar{1}]$

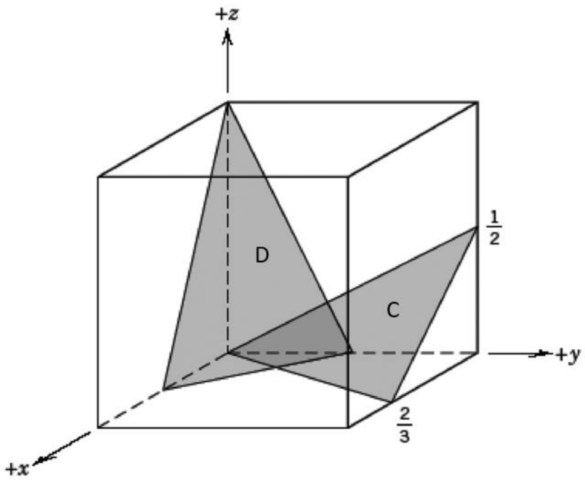
B: $[\bar{2}10]$

C: $[1\bar{3}\bar{3}]$

D: $[13\bar{6}]$

9. Determine the Miller indices for the planes shown in the following cubic unit cell





A: $(32\bar{2})$.
B: $(\bar{1}01)$
C: $(3\bar{2}4)$
D: (221)

10. Find a direction that is the intersection of the planes $(41\bar{2})$ and $(\bar{2}12)$ in a cubic structure. Hint: (hkl) is perpendicular to [uvw] in cubic crystal structures.

For cubic, $[41\bar{2}] \perp (41\bar{2})$ and $[\bar{2}12] \perp (\bar{2}12)$. The intersection of $(41\bar{2})$ and $(\bar{2}12)$ can be found by the cross-product of $[41\bar{2}]$ and $[\bar{2}12]$.

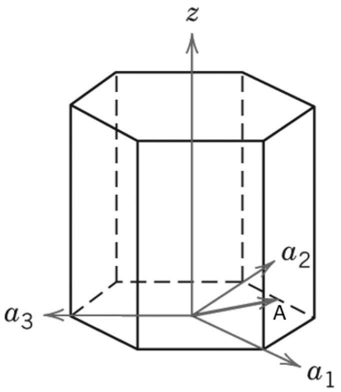
$$[41\bar{2}] \times [\bar{2}12] = \begin{vmatrix} i & j & k \\ 4 & 1 & -2 \\ -2 & 1 & 2 \end{vmatrix} = (2+2)i - (8-4)j + (4+2)k = 4i - 4j + 6k$$

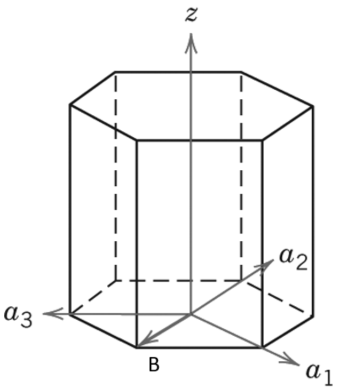
Therefore the direction is $[2\bar{2}3]$

11. Identify close packed planes and close packed directions in body centered cubic, face centered cubic, and hexagonal close packed structures. Use Miller-Bravais indices for the hexagonal system.

- BCC: The close packed planes are the {110} family, which includes $(110), (101), (011), (\bar{1}10), (10\bar{1}), (1\bar{1}0)$. The close packed directions are the <111> family, which includes $[111], [\bar{1}11], [1\bar{1}1], [11\bar{1}]$.
- FCC: The close packed planes are the {111} family, which includes $(111), (\bar{1}11), (1\bar{1}1), (11\bar{1})$, The close packed directions are the <110> family, which includes $[110], [101], [011], [\bar{1}10], [01\bar{1}], [10\bar{1}]$.
- HCP: the close packed plane is the basal plane (0001). The close packed directions are the $<11\bar{2}0>$ family, which includes $[11\bar{2}0]$, $[\bar{2}110]$, $[1\bar{2}10]$.

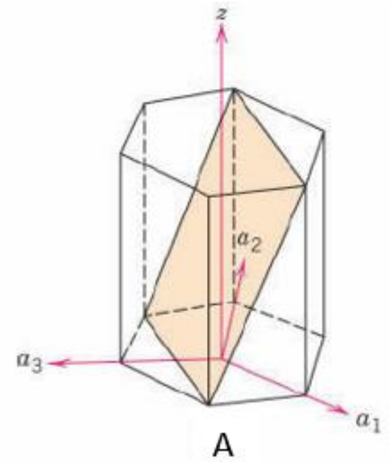
12. (a) Determine the indices for the directions shown in the following hexagonal unit cells

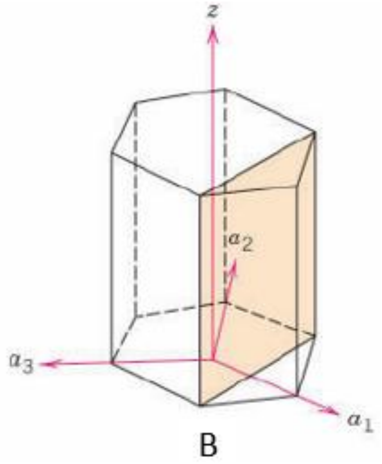




A: $[01\overline{1}0]$
B: $[1\overline{2}10]$

(b) Determine the indices for the planes shown in the following hexagonal unit cells





A: $(\overline{11}22)$
B: $(2\overline{11}0)$

13. Would you expect a material in which the atomic bonding is predominantly ionic in nature to be more likely or less likely to form a noncrystalline solid upon solidification than a covalent material? Why?

The ionically bonded material is less likely to form a noncrystalline solid.

By definition, ionic bonding heavily favors unlike ions neighboring each other. The energy required to disorder the system and have liked charged neighbors is thus prohibitively large. Further, ionic bonds are nondirectional, whereas covalent bonds are directional. The directional nature of the bonds makes it difficult to align many molecules in an orderly fashion, resulting in a tendency to form noncrystalline solids (see the structure of crystalline and amorphous SiO2, Figure 3.25).