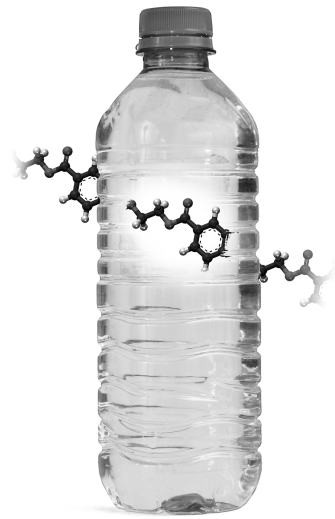


HOMework 2.

solutions



Practice Problems

1. Askeland Problem 2-23. Materials such as silicon carbide (SiC) and silicon nitride (Si₃N₄) are used for grinding and polishing applications. Rationalize the choice of these materials for this application (discuss structure-property connections).

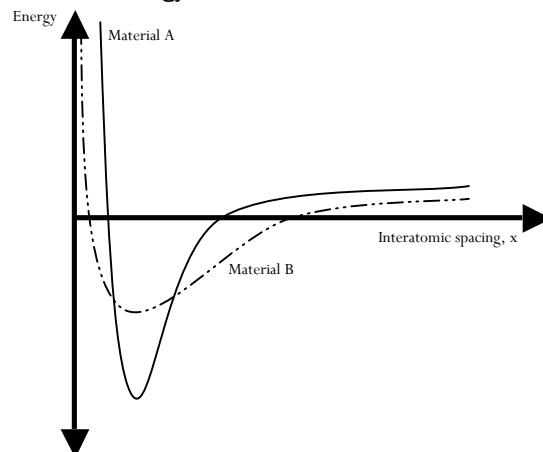
Silicon carbide and silicon nitride exhibit primarily covalent bonding. As a result, SiC and Si₃N₄ are very hard, very strong, and very brittle materials, and they have high melting temperatures. What properties would you like in a grinding material? Grinding and polishing involve lots of plastic deformation, so you need a grinding material that is harder and stronger than the material you are grinding or polishing. The brittleness of silicon carbide and silicon nitride enable the formation of sharp, angular grinding particles. The high melting temperature of silicon carbide and silicon nitride helps, too, since many grinding and polishing processes result in significant heating at the ground surface.

2. Askeland Problem 2-32. Would you expect Al₂O₃ or aluminum to have a higher coefficient of thermal expansion? Explain.

2-32 Would you expect Al₂O₃ or aluminum to have the higher coefficient of thermal expansion? Explain.

Solution: Al₂O₃ has stronger bonds than Al; therefore, Al₂O₃ should have a lower thermal expansion coefficient than Al. In Al, $\alpha = 25 \times 10^{-6} \text{ cm/cm}^\circ\text{C}$; in Al₂O₃, $\alpha = 6.7 \times 10^{-6} \text{ cm/cm}^\circ\text{C}$.

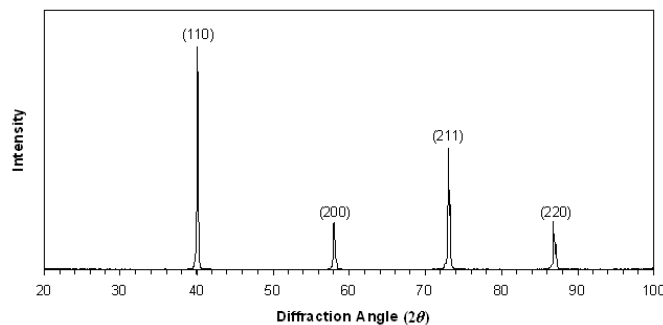
3. Consider the following graph of the bond-energy curves for two different materials.



- a. Which of the two materials will have the lowest coefficient of thermal expansion over a given change in temperature? Justify your answer.
Material (a) would have lower thermal expansion than material (b). As temperature is increased (thermal energy is added), the average interatomic spacing (given by x') in material (a) shows less of an increase than the average interatomic spacing in material (b).
- b. Which of the two materials will have a higher melting temperature? Justify your answer.
Material (a) would exhibit a higher melting temperature. The energy well (depth of the E vs. r curve) is much greater for Material A, so it will take a lot more energy to disrupt the bonding and separate the atoms, as we'd need to do if we wanted to melt the materials.
- c. Which of the two materials will have a higher stiffness? Justify your answer.
Material (a) would exhibit a higher stiffness. Stiffness is related to the force required to displace atoms from their equilibrium positions. To get a sense of the stiffness, we should take the derivative of the E vs. r curve and generate a Force vs. interatomic separation curve. If we did this, the slope of the F vs. r curve for Material A would be much steeper (take a look at the change in curvature at the bottom of the energy well). Thus, it would require more force to pull atoms apart...higher stiffness.
- d. If Material B is a metal, do you think that Material A is a metal, ceramic, or polymer? Justify your answer.
 Hey, this is an interesting question! Compared to Material B, Material A has a higher melting temperature, higher stiffness, and lower thermal expansion. It sounds like a **ceramic** material to me. It could also be a **different metal**. For example, if Material B is aluminum, Material B could be tungsten.

4. An unforeseeable reaction has just destroyed the metal lining of your high temperature vacuum furnace. You can't afford to purchase a new lining, so you've decided to make a new lining in the Olin shop. The lining is basically a 6-inch metal cube with a wall thickness of 0.125 inches. One problem: you don't know the material used for the furnace lining. You think you can safely assume it's a pure metal, but other than that, you're at a loss.

To determine the unknown metal, you run a standard x-ray diffraction scan, the results of which are shown in the following figure. Crystallographic planes (hkl) are indexed on the pattern. The copper radiation used in the x-ray diffraction test had a wavelength of 0.1542 nm.



- a. Given the XRD data, what is the likely crystal structure of the unknown metal?
- To determine the structure of the metal, we need to observe the (hkl) values shown on the plot and compare the values to the allowed (hkl) values for common metals. Careful observation of the data shows that the sum of each set of (hkl) is an even number, or $h+k+l=\text{even}$. From the class notes or the XRD section on the Callister CD-ROM, we know that the body centered cubic (bcc) structure common to many metals has $h+k+l=\text{even}$. Thus, we can assume this XRD pattern is from a **metal with a bcc structure**.
- b. What is the lattice parameter of the unknown metal?
- To determine the lattice parameter of this bcc metal, we may select any of the indexed (hkl) diffraction peaks. Let's pick the first x-ray peak at about $2\theta=40^\circ$ corresponding to the (110) planes in the metal. The first step in determining the lattice parameter is to calculate the interplanar spacing (d-spacing) for the (110) planes, as follows:

$$d_{(110)} = \frac{n\lambda}{2 \sin(\theta)} = \frac{(1)(0.1542 \text{ nm})}{2 \sin(20^\circ)} = 0.225 \text{ nm}$$

Now we need to determine the lattice parameter “a” from this d-spacing:

$$a = d_{(hkl)} \sqrt{h^2 + k^2 + l^2} = 0.225 \text{ nm} \sqrt{1^2 + 1^2 + 0^2} = 0.319 \text{ nm}$$

c. Based on your answers in parts (a) and (b), which of the following materials is the most likely match for the unknown metal?

- i. Tantalum
- ii. Nickel
- iii. Sodium
- iv. Zirconium
- v. Tungsten
- vi. Chromium

o Since we have already assumed we have a bcc structure, we can calculate the atomic radius from our lattice parameter a to atomic radius R relationship for the bcc structure:

$$a = \frac{4R}{\sqrt{3}}$$

$$R = \frac{a\sqrt{3}}{4} = \frac{0.319 \text{ nm} \sqrt{3}}{4} = 0.138 \text{ nm}$$

Of the metals in the list, **tungsten** is the best match with our bcc structure and approximate 0.138 nm atomic radius requirements.

d. Will you be able to fabricate the material in the Olin machine shop? Briefly explain your answer.

o Interesting question! What do we know about tungsten? It's a metal with a high melting temperature, which indicates strong interatomic bonding. The Callister appendices tell us that tungsten has a really high yield strength and modulus of elasticity compared to most metals and alloys. I would expect that machining tungsten is fairly difficult. You would probably want to use carbide tools, which are actually tungsten carbide ceramic-like particles in a metal matrix, rather than more common high speed steel tools.

5. Noncrystalline SiO₂ is optically transparent. Polycrystalline SiO₂ is opaque or translucent. Single crystal SiO₂ is optically transparent. Explain.

o In polycrystalline SiO₂, the crystallographic orientation of individual grains will be different. The different crystallographic orientations will provide a slightly different index of refraction between grains, and reflection and refraction of light at grain boundaries will result, leading to translucency or opacity. Single crystal and noncrystalline (amorphous) SiO₂ will have the same structure/orientation throughout the material providing for easy transmission of light. Note that some single crystals and noncrystalline ceramics and glasses are translucent or opaque to visible light due to other factors (e.g., scattering of light by porosity or impurities, absorption of radiation by electron transitions, etc.).

6. Askeland Problem 3-34. Beryllium has a hexagonal crystal structure, with a₀ = 0.22858 nm and c₀ = 0.35842 nm. The atomic radius is 0.1143 nm, the density is 1.848 g/cm³, and the atomic weight is 9.01 g/mol. Determine

- a. The number of atoms in each unit cell; and
- b. The packing factor in the unit cell

Solution: $V = (0.22858 \text{ nm})^2(0.35842 \text{ nm})\cos 30 = 0.01622 \text{ nm}^3 = 16.22 \times 10^{-24} \text{ cm}^3$

(a) From the density equation:

$$1.848 \text{ g/cm}^3 = \frac{(x \text{ atoms/cell})(9.01 \text{ g/mol})}{(16.22 \times 10^{-24} \text{ cm}^3)(6.02 \times 10^{23} \text{ atoms/mol})}$$

$$x = 2 \text{ atoms/cell}$$

(b) The packing factor (PF) is:

$$\text{PF} = \frac{(2 \text{ atoms/cell})(4\pi/3)(0.1143 \text{ nm})^3}{0.01622 \text{ nm}^3} = 0.77$$

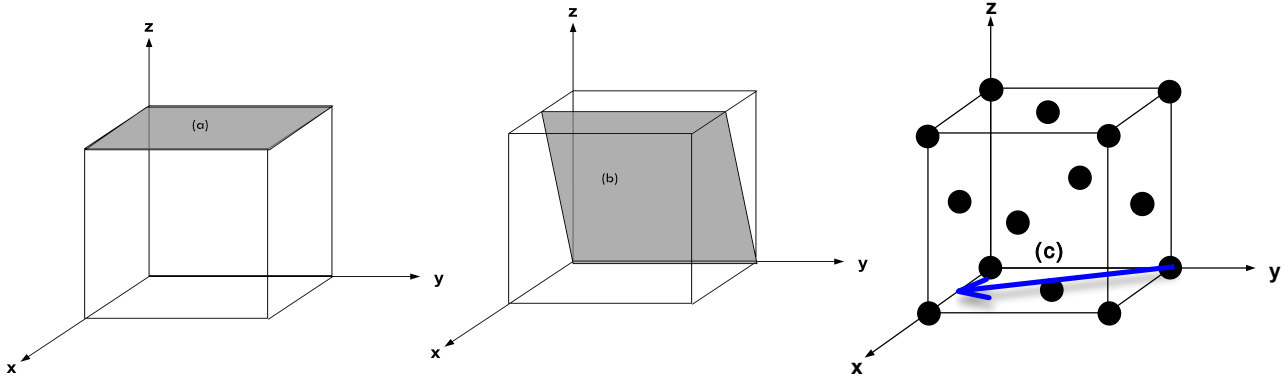
7. Askeland Problem 3-78. Explain why most often polycrystalline materials exhibit isotropic properties.

Most polycrystalline materials consist of randomly arranged crystals or “grains.” Although individual grains have different orientations and behave anisotropically by themselves, at a larger scale the material behavior is determined by the sum of many grain orientations, and the bulk material acts in an isotropic manner. There are some notable exceptions to this generalization. If the crystals or grains in a solid material are all aligned in the same or similar directions (called “columnar” orientation of grains), as is the case in some turbine blades, the crystal will exhibit anisotropic behavior.

8. Crystallographic planes. Sketch an fcc unit cell. Within the unit cell, sketch and label the following:

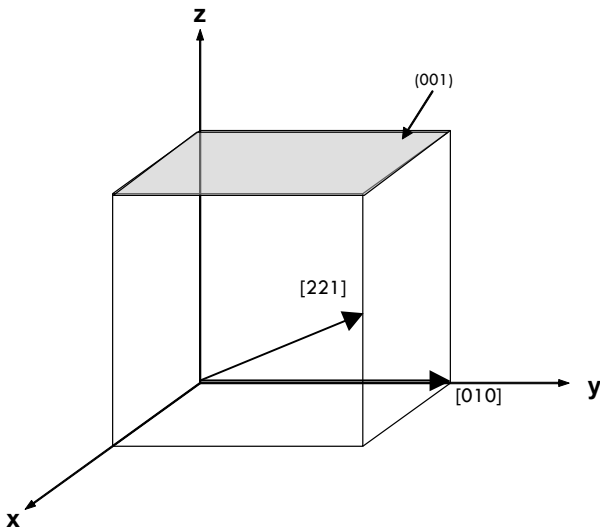
- a. (001) b. $(20\bar{1})$ c. $[\bar{1}\bar{2}0]$

Well, I didn't include the atomic positions in all these sketches, but I think you get the idea...



9. Crystallographic planes and directions. Sketch a bcc unit cell. Within the unit cell, sketch and label the following:

- b. $[010]$ b. $[221]$ c. (001)



10. Nickel has the fcc structure and a lattice parameter of $a = 0.3517 \text{ nm}$.

c. Determine the atomic radius in nm. Compare this value to that shown in the front of your textbook.

o $R = a/(2\sqrt{2}) = \mathbf{0.124 \text{ nm}}$

d. Determine the atomic volume Ω in nm^3 (assume a spherical atom shape).

o Assuming a spherical atoms, $\Omega = 4\pi R^3/3 = .000805 \text{ nm}^3 = \mathbf{8.05 \times 10^{-3} \text{ nm}^3}$

e. Determine the density in g/cm^3 and compare this answer to the Ni density value given in the table at the front of your textbook.

$$r = \frac{nA}{V_c N_A} = \frac{4 \text{ atoms/cell} \cdot 58.693 \text{ g/mol}}{(0.3517 \text{ nm})^3 \cdot (6.023 \times 10^{23} \text{ atoms/mol})} = 8.96 \times 10^{-21} \text{ g/nm}^3 = 8.96 \text{ g/cm}^3$$

o Book value for nickel density is 8.90 g/cm^3 , so the values are very close (hard sphere model is pretty good).

11. Sketch an fcc unit cell.

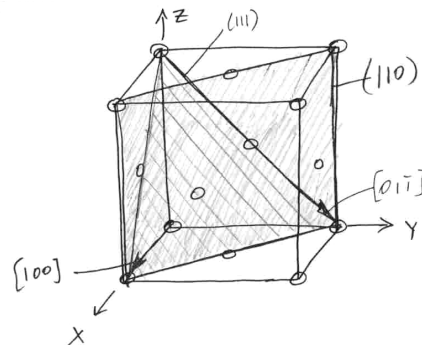
f. Determine the planar density for the (111) .

g. Determine the planar density for the (110) .

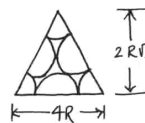
h. Determine the linear density for the $[01\bar{1}]$

i. Determine the linear density for the $[100]$.

j. Given the densities you calculated for (a)-(d), which planes and directions would provide the easiest path for edge dislocation motion, or "slip"?



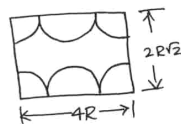
(a) (111) PLANAR DENSITY



$$3 \cdot \frac{1}{6} + 3 \cdot \frac{1}{2} = 2 \text{ ATOMS}$$

$$PD = \frac{\text{AREA OF ATOMS}}{\text{AREA OF PLANE}} = \frac{2 \text{ ATOMS} \cdot \pi R^2}{4R^2 \sqrt{3}} = \underline{\underline{0.907}}$$

(b) (110) PLANAR DENSITY



$$PD = \frac{2 \text{ ATOMS} \cdot \pi R^2}{8R^2 \sqrt{2}} = \underline{\underline{0.555}}$$

(c) $[01\bar{1}]$ LINEAR DENSITY

$$LD = \frac{\text{LINE LENGTH OF ATOMS}}{\text{TOTAL LINE LENGTH}} = \frac{4R}{4R\sqrt{2}} = \frac{4R}{4R} = \underline{\underline{1}}$$

(d) $[100]$ LINEAR DENSITY

$$LD = \frac{2R}{a} = \frac{2R}{2R\sqrt{2}} = \frac{1}{\sqrt{2}} = \underline{\underline{0.707}}$$