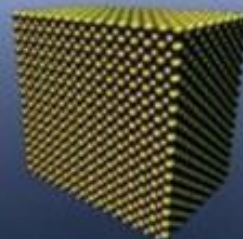
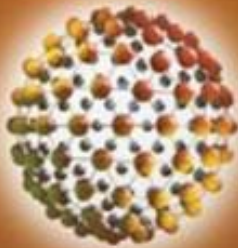


SOLUTIONS MANUAL

SI EDITION

Second Edition

Essentials of Materials Science and Engineering



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CHAPTER 2 ATOMIC STRUCTURE

2-6(a) Aluminum foil used for storing food weighs about 0.05 g/cm². How many atoms of aluminum are contained in this sample of foil?

Solution: *In a one square centimeter sample:*

$$\text{number} = \frac{(0.05 \text{ g})(6.02 \times 10^{23} \text{ atoms/mol})}{26.981 \text{ g/mol}} = 1.037 \times 10^{21} \text{ atoms}$$

2-6(b) Using the densities and atomic weights given in Appendix A, calculate and compare the number of atoms per cubic centimeter in (a) lead and (b) lithium.

Solution: (a) *In lead:*

$$\frac{(11.36 \text{ g/cm}^3)(1 \text{ cm}^3)(6.02 \times 10^{23} \text{ atoms/mol})}{207.19 \text{ g/mol}} = 3.3 \times 10^{22} \text{ atoms/cm}^3$$

(b) *In lithium:*

$$\frac{(0.534 \text{ g/cm}^3)(1 \text{ cm}^3)(6.02 \times 10^{23} \text{ atoms/mol})}{6.94 \text{ g/mol}} = 4.63 \times 10^{22} \text{ atoms/cm}^3$$

2-7(a) Using data in Appendix A, calculate the number of iron atoms in one ton (1000 kilograms) of iron.

Solution:

$$\frac{(1000 \times 10^3)(6.02 \times 10^{23} \text{ atoms/mol})}{55.847 \text{ g/mol}} = 1.078 \times 10^{28} \text{ atoms/ton}$$

2-7(b) Using data in Appendix A, calculate the volume in cubic centimeters occupied by one mole of boron.

Solution:

$$\frac{(1 \text{ mol})(10.81 \text{ g/mol})}{2.3 \text{ g/cm}^3} = 4.7 \text{ cm}^3$$

2-8 In order to plate a steel part having a surface area of 1250 cm² with a 0.005 cm thick layer of nickel, (a) how many atoms of nickel are required and (b) how many moles of nickel are required?

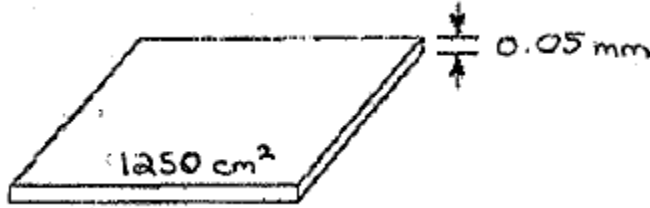
Solution: Volume = (1250 cm²)(0.005 cm) = 6.25 cm³

(a)

$$\frac{(6.25 \text{ cm}^3)(8.902 \text{ g/cm}^3)(6.02 \times 10^{23} \text{ atoms/mol})}{58.71 \text{ g/mol}} = 5.70 \times 10^{23}$$

(b)

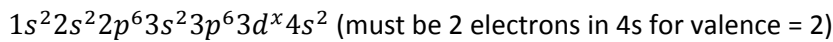
$$\frac{(6.25 \text{ cm}^3)(8.902 \text{ g/cm}^3)}{58.71 \text{ g/mol}} = 0.948 \text{ mol Ni required}$$



2-9 Suppose an element has a valence of 2 and an atomic number of 27. Based only on the quantum numbers, how many electrons must be present in the 3d energy level?

Solution: *We can let x be the number of electrons in the 3d energy level.*

Then:



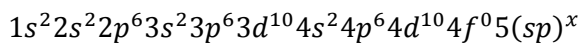
$$\text{Since } 27 - (2 + 2 + 6 + 2 + 6 + 2) = 7 = x$$

There must be 7 electrons in the 3d level.

2-10 Indium, which has an atomic number of 49, contains no electrons in its 4f energy level. Based only on this information, what must be the valence of indium?

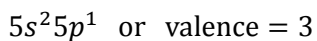
Solution: *We can let x be the number of electrons in the outer sp energy level.*

Then:



$$49 - (2 + 2 + 6 + 2 + 6 + 10 + 2 + 6 + 10 + 0) = 3$$

Therefore the outer 5sp level must be:



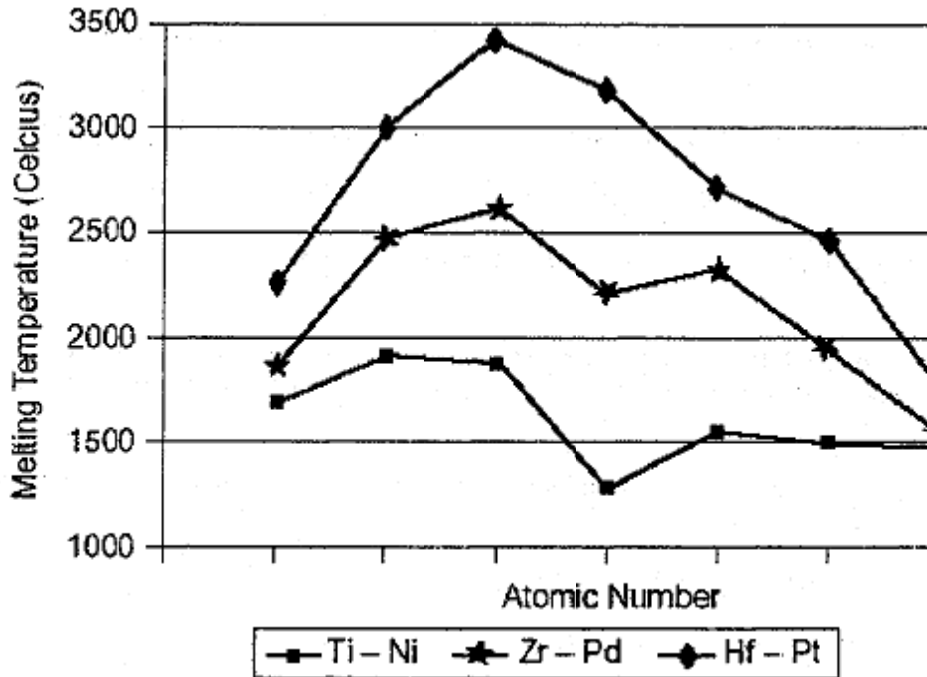
2-12 Bonding in the intermetallic compound Ni₃Al is predominantly metallic. Explain why there will be little, if any, ionic bonding component. The electronegativity of nickel is about 1.9.

Solution: *The electronegativity of Al is 1.5, while that of Ni is 1.9. These values are relatively close, so we wouldn't expect much ionic bonding. Also, both are metals and prefer to give up their electrons rather than share or donate them.*

2-13 Plot the melting temperatures of elements in the 4A to 8-10 columns of the periodic table versus atomic number (that is, plot melting temperatures of Ti through Ni, Zr through Pd, and Hf through Pt). Discuss these relationships, based on atomic bonding and binding energy, (a) as the atomic number increases in each row of the periodic table and (b) as the atomic number increases in each column of the periodic table.

Solution:

Ti – 1668	Zr – 1852	Hf – 2227
V – 1900	Nb – 2468	Ta – 2996
Cr – 1875	Mo – 2610	W – 3410
Mn – 1244	Tc – 2200	Re – 3180
Fe – 1538	Ru – 2310	Os – 2700
Co – 1495	Rh – 1963	Ir – 2447
Ni – 1453	Pd – 1552	Pt – 1769

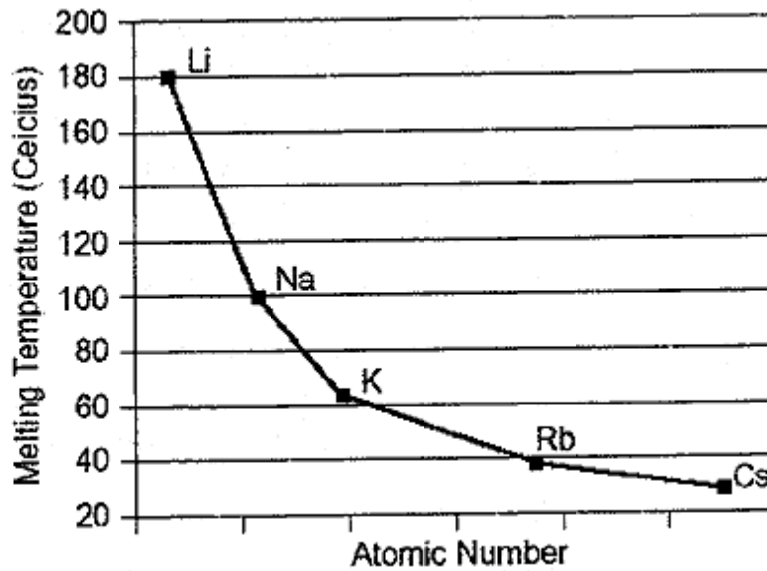


For each row, the melting temperature is highest when the outer “d” energy level is partly full. In Cr, there are 5 electrons in the 3d shell; in Mo, there are 5 electrons in the 4d shell; in W there are 4 electrons in the 5d shell. In each column, the melting temperature increases as the atomic number increases – the atom cores contain a larger number of tightly held electrons, making the metals more stable.

2-14 Plot the melting temperature of the elements in the 1A column of the periodic table versus atomic number (that is plot melting temperature of Li through Cs). Discuss this relationship, based on atomic bonding and binding energy.

Solution:

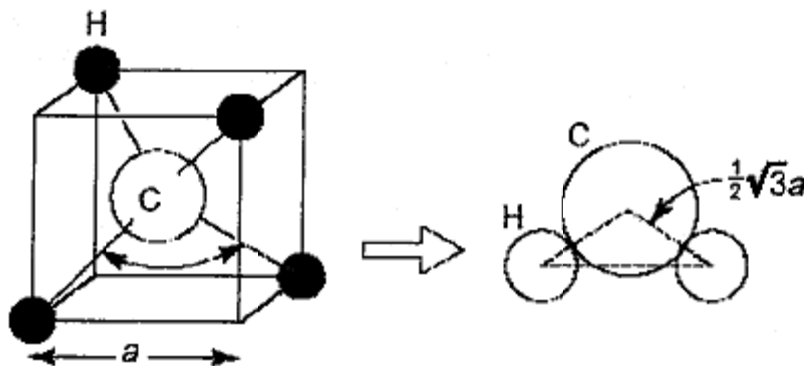
<u>T(°C)</u>
Li – 180.7
Na – 97.8
K – 63.2
Rb – 38.9
Cs – 28.6



As the atomic number increases, the melting temperature decreases, opposite that found in problem 2-13.

- 2-15 Methane (CH_4) has a tetrahedral structure similar to that of SiO_2 , with a carbon atom of radius 0.77×10^{-8} cm at four of the eight corners. Calculate the size of the tetrahedral cube for methane.

Solution:



- 2-16 The compound (AlP) is a compound semiconducting material having mixed ionic and covalent bonding. Estimate the fraction of the bonding that is ionic.

Solution: $E_{A1} = 1.5$ $E_P = 2.1$

$$f_{\text{covalent}} = \exp(0.25 \Delta E^2)$$

$$f_{\text{covalent}} = \exp[(0.25)(2.1 - 1.5)^2] = \exp[-0.09] = 0.914$$

$$f_{\text{ionic}} = 1 - 0.914 = 0.086 \therefore \text{bonding is mostly covalent}$$

2-17 Calculate the fraction of bonding of MgO that is ionic.

Solution: $E_{Mg} = 1.2$ $E_O = 3.5$

$$f_{\text{covalent}} = \exp[(-0.25)(3.5 - 1.2)^2] = \exp(-1.3225) = 0.266$$

$$f_{\text{ionic}} = 1 - 0.266 = 0.734 \therefore \text{bonding is mostly ionic}$$

2-21 Calculate the fractions of ionic bonds in silicon carbide (SiC) and in silicon nitride (Si₃N₄).

Solution: *Fraction covalent* = $\exp(-0.25(\Delta E)^2)$

$$\text{For silicon nitride: Fraction covalent} = \exp(-0.25(2.6-1.8)^2) = 0.69 \text{ or } 69\%$$

$$\text{For silicon carbide fraction covalent} = \exp(-0.25(3.0-1.8)^2) = 0.85 \text{ or } 85\%$$

2-22 One particular form of boron nitride (BN) known as cubic boron nitride (CBN) is a very hard material and is used in grinding applications. Calculate the fraction of covalent bond character in this material.

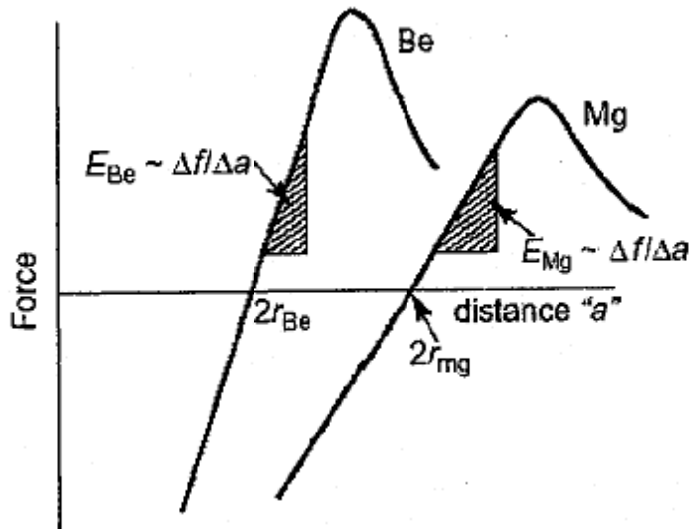
Solution: *For boron nitride fraction covalent* = $\exp(-0.25(3.0-2.0)^2) = 0.78 \text{ or } 78\%$

2-23 Another form of boron nitride (BN), however, known as hexagonal boron nitride (HBN) is used as a solid lubricant. Explain, how this may be possible by comparing this situation with that encountered in two forms of carbon namely diamond and graphite.

Solution: *When crystal structure of a material is considered i.e. we look for atomic arrangements beyond simply the bond between two atoms, we can see that atoms or ions may be arranged in layered arrangements. The bonds between layers are often van der Waals and hence it is possible to apply a shearing force that results in cleaving of the different planes of atoms. Hexagonal boron nitride has graphite like structure and is known as "white graphite" and it used as a solid lubricant. Cubic boron nitride, on the other hand, has diamond cubic structure and is hard similar to diamond and is used in cutting tools.*

2-24 Beryllium and magnesium, both in the 2A column of the periodic table, are lightweight metals. Which would you expect to have the higher modulus of elasticity? Explain, considering binding energy and atom radii and using appropriate sketches of force versus interatomic spacing.

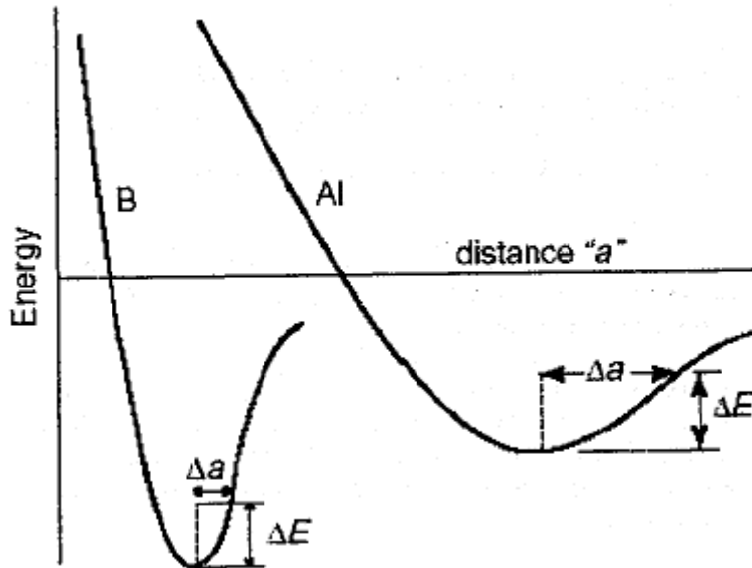
Solution:



The smaller Be electrons are held closer to the core \therefore held more tightly, giving a higher binding energy.

- 2-25 Boron has a much lower coefficient of thermal expansion than aluminum, even though both are in the 3B column of the periodic table. Explain, based on binding energy, atomic size, and the energy well, why this difference is expected.

Solution:



Electrons in Al are not as tightly bonded as those in B due to the smaller size of the boron atom and the lower binding energy associated with its size.

2-26 Would you expect MgO or magnesium to have the higher modulus of elasticity? Explain.

Solution: *MgO has ionic bonds, which are strong compared to the metallic bonds in Mg. A higher force will be required to cause the same separation between the ions in MgO compared to the atoms in Mg. Therefore, MgO should have the higher modulus of elasticity. In Mg, ; in MgO,*

2-27 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, ; in Al₂O₃,*

2-28 Aluminum and silicon are side-by-side in the periodic table. Which would you expect to have the higher modulus of elasticity (E)? Explain.

Solution: *Silicon has covalent bonds; aluminum has metallic bonds. Therefore, Si should have a higher modulus of elasticity.*

2-29 Explain why the modulus of elasticity of simple thermoplastic polymers, such as polyethylene and polystyrene, is expected to be very low compared with that of metals and ceramics.

Solution: *The chains in polymers are held to other chains by Van der Waals bonds, which are much weaker than metallic, ionic, and covalent bonds. For this reason, much less force is required to shear these weak bonds and to unkink and straighten the chains.*

2-30 Steel is coated with a thin layer of ceramic to help protect against corrosion. What do you expect to happen to the coating when the temperature of the steel is increased significantly? Explain.

Solution: *Ceramics are expected to have a low coefficient of thermal expansion due to strong ionic/covalent bonds; steel has a high thermal expansion coefficient. When the structure heats, steel expands more than the coating, which may crack and expose the underlying steel to corrosion.*

2-32 An aluminum-alloy bar of length 2 meters at room temperature (300 K) is exposed to a temperature of 100 C ($\alpha = 23 \times 10^{-6} \text{ K}^{-1}$). What will be the length of this bar at 100 C?

Solution: *Assume the starting temperature is 300 K.*

$$\alpha = \left(\frac{1}{L} \right) \left(\frac{dL}{dT} \right)$$

$$23 \times 10^{-6} = \left(\frac{1}{2\text{m}} \right) \left(\frac{dL}{(373 - 300)\text{K}} \right)$$

Thus, the change in length (dL) will be = 0.3358 cm. or 3.3358 mm.

2- 33 If the elastic modulus of the aluminum alloy in the example above is $70 \times 10^9 \text{ N/m}^2$ (or Pa), what will be stress generated in the aluminum alloy bar heated to 100 C, if the bar was constrained between rigid supports and thus not allowed to expand? Will this stress be compressive or tensile in nature?

Solution: $\sigma = \alpha \times \Delta T \times E$
 $\sigma = (23 \times 10^{-6} \text{ K}^{-1}) \times (373 - 300) \times (70 \times 10^9 \text{ Pa}) = 1.18 \times 10^8 \text{ Pa}$

The bar wants to expand and is prevented from doing so, because of the rigid constraints, thus effectively a compressive stress is being applied to the bar.

2-36 You want to design a material for making a mirror for a telescope that will be launched in space. Given that the temperatures in space can change considerably. What material will you consider using? Remember that this material should not expand or contract at all, if possible. It should also be as strong and also as low density as possible and one should be able to coat it so that it can serve as a mirror.

Solution: *Temperatures encountered in space vary considerably. Similarly, even for ground based telescopes located on high mountain tops temperatures can be low (~ - 40 C). A major consideration for selecting materials for telescope mirrors is low coefficient of thermal expansion. Schott Glass corporation has developed a material called Zerodur (see Chapter 15) that has essentially zero thermal expansion coefficient. The material can be coated on one side to provide a mirror surface. It is also low density (~ 2.5 g/cc).*

- 2-37 You want to use a material that can be used for making a catalytic converter substrate. The job of this material is to be a carrier for the nanoparticles of metals such as platinum and palladium which are the actual catalysts. The main considerations are that this catalyst support material must be able to withstand the constant, cyclic heating and cooling that it will be exposed to. The gases from automobile exhaust reach temperatures up to 500 C and the material will get heated up to high temperatures and then cool down when the car is not being used. What kinds of materials can be used for this application?

Solution: *A major consideration in selecting a material for this application would be whether there is sufficient thermal shock resistance. This means as the material gets repeatedly heated to a few hundred degrees centigrade and cools down will the thermal stresses caused by thermal expansion and contraction cause the material to fail. Secondly, the material should be inert in that it should not react with the nanoparticles of Pt/Pd/Rh that function as a catalyst. Inertness also means that the catalytic substrate itself should be able to withstand the reducing and oxidizing chemical environments it will be exposed to. Thus, most metallic materials can be ruled out on the basis of chemical inertness. Most polymers will not be able to withstand the temperatures. Also the thermal coefficient of most polymers is relatively large. Thus, the choice may be mainly between ceramic materials. Regular inorganic glasses will not work because of the thermal expansion coefficient is too high and repeated heating and cooling will cause them to fracture. Thus, ceramics such as alumina, zirconia etc. may work, a key would also be there should be no phase transformation or change in crystal structure that causes an abrupt volume changes. Over a period of time a material of choice is a ceramic material known as cordierite ($Mg_2Al_4Si_5O_{18}$). This is a magnesium aluminosilicate. It has a small thermal expansion coefficient ($\sim 4 \times 10^{-7}/^{\circ}C$), it is relatively stable and not too expensive. The catalytic converter substrates are manufactured using a process known as ceramic extrusion and in using this process we take advantage of the anisotropy of thermal expansion of cordierite.*

- 2-40 Solid Oxide Fuel Cell Materials: A solid oxide fuel cell is made using a thin film of yttria stabilized zirconia (ZrO_2) (YSZ). The film is deposited onto a ceramic tube of a material called strontium (Sr) doped lanthanum manganite ($LaMnO_3$) (known as LSM). On the zirconia ceramic film another layer of nickel is deposited and serves as the anode. The LSM material acts as a cathode. The thermal expansion coefficient of YSZ used here was $10 \times 10^{-6} C^{-1}$. The thermal expansion coefficient of nickel is $13.3 \times 10^{-6} C^{-1}$. What type of stress will the nickel film be subjected to, if we assume that both YSZ and LSM used here have very similar thermal expansion coefficients? What will be the magnitude of the stress in nickel film?

Solution: *Nickel has higher coefficient of expansion than YSZ/LSM used here, thus it would like to expand more. However, it is constrained by the YSZ/LSM. Thus, the nickel film, assumed to be grown at higher temperatures, wants to shrink but is not allowed and hence the nickel film is subjected to a tensile stress. However, nickel film is not free it is attached to ZrO_2 /LSM substrate and as this composite structure heats and cools down, the ZrO_2 /LSM also expands and contracts, thus the actual stress developed in nickel film will be:*

$$\sigma = \Delta\alpha \times \Delta T \times E$$

where $\Delta\alpha$ is the difference in the coefficients of thermal expansion of the film and the substrate. What this says is that if the film and substrate thermal expansion coefficients match (i.e. $\Delta\alpha=0$), then there is no stress developed in the film. Assume that nickel elastic modulus is 160 GPa.

Thus, substituting actual tensile stress developed in nickel thin film will be $= 4.22 \times 10^8$ Pa. This does not account for the Poisson's ratio effects.