Problem Set 3
Due: Tuesday, February 7, 11:00 AM

1. Yield/Shear on Storke Tower
Suppose the largest bell in Storke Tower, which weighs 4,793 pounds, needs to be replaced. A crane is brought in to remove the bell, initially using a 304 Stainless Steel cable that is 0.551 inches in diameter. The cable is arranged such that a length of 9’10.1” of steel is bearing the weight of the bell. The yield strength of 304SS is 205 MPa from Callister Table 11.4, and the Young’s modulus is 193 GPa, from azom.com. (Note: Use metric units when solving the problems. Problem adapted from Prof. Van Vliet, 3.032.)

a) i) Will the cable yield to the weight of the bell? (12 pts total)

The weight of the bell in kilograms is ~2,174. The radius is about 7mm or 0.007 m.

\[ \text{Stress, } \sigma = \frac{F}{A} = \frac{ma}{\pi r^2} = \frac{2,174 \text{ kg} \times 9.8 \text{ m/s}^2}{\pi (0.007 \text{ m})^2} = \frac{21,305 \text{ N}}{1.5394 \times 10^{-4}} = 138.4 \text{ MPa} \]

\[ \sigma = 138.4 \text{ MPa} < 205 \text{ MPa} = \sigma_y \]

The cable will not yield.

ii) What is the maximum load (in N) that the cable can withstand before yielding?

The maximum load it can withstand is

\[ \sigma_y = 205 \text{ MPa} = \frac{F_{\text{max}}}{A} = \frac{F_{\text{max}}}{1.54 \times 10^{-4} \text{ m}^2} \Rightarrow F_{\text{max}} = 31,557.3 \text{ N} \]

iii) If it does not yield, then what is the displacement (in mm) of the bell as the cable deforms elastically?

The elastic deformation will cause a strain of:

\[ \sigma = E \varepsilon \Rightarrow \varepsilon = \frac{\sigma}{E} = \frac{138.4 \text{ MPa}}{193 \text{ GPa}} = 7.171 \times 10^{-4} \]

The length of the steel is 9 feet, 10.1 inches, or 3 meters.

\[ \delta_z = \varepsilon L_0 = 7.171 \times 10^{-4} \times 3 \text{ m} \approx 2.15 \text{ mm} \]

b) What is the maximum sheer stress in the cable while carrying this bell? (2 pts)

Using the Schmidt factor, and knowing that maximum stress occurs at 45° to the loading direction,

\[ \tau = \sigma \cos \theta \sin \theta = 138.4 \text{ MPa} \times \cos(45) \sin(45) = 69.2 \text{ MPa} \]

c) The University requested that the company use a cable of sufficient thickness to have a safety factor of 4. The crane’s pulley system can only accommodate a cable of 0.75” diameters or less. If the company does not wish to use a wider set of pulleys, will they be able to meet the requirement with 304 SS cable? (6 pts)
To get a safety factor of 4, the maximum tensile stress on the cable is as below. This leads to a minimum cross-sectional area for the cable before yielding occurs.

\[
\sigma_{\text{w}} = \frac{\sigma_y}{4} = 51.25 \text{ MPa} = \frac{F_{\text{bell}}}{A_{\text{min}}} = \frac{21305 \text{ N}}{A_{\text{min}}} \Rightarrow A_{\text{min}} = \frac{21305 \text{ N}}{51.25 \text{ MPa}} = 4.16 \times 10^{-4} \text{ m}^2
\]

This means the cable must have a diameter of

\[
A_{\text{min}} = \pi \left(\frac{d_{\text{min}}}{2}\right)^2 \Rightarrow d_{\text{min}} = 2 \sqrt{\frac{A_{\text{min}}}{\pi}} = 2 \sqrt{\frac{4.16 \times 10^{-4} \text{ m}^2}{\pi}} = 0.023 \text{ m} \times \frac{39.37 \text{ in}}{\text{m}} = 0.905 \text{ in}
\]

This is wider than the pulley groove. 304 SS won’t meet the requirement.

2. Defects in ceramics (Callister 12.5): SrTiO$_3$

By now we should all be somewhat familiar with the perovskite structure SrTiO$_3$.

a) Featured below is a TiO$_2$ plane for a very poor sample of SrTiO$_3$. Give the miller index of this plane with respect to Figure 12.6 of Callister. In the figure below, label all the point defects present. You should find at least one of the following: Cation vacancy, anion vacancy, cation interstitial, anion interstitial, Frenkel defect, Schottky defect, substitutional impurity, and interstitial impurity. **Note: Frenkel and Schottky defects involve more than one point defect in close proximity to one another, while other point defects can be isolated. (8 pts)**
b) Of these types of defects, which will alter the stoichiometry of the sample, and which will preserve it? (2 pts)

The cation to anion ratio within a sample is not effected by the presence of Frenkel and Schottky defects. Therefore, stoichiometry is preserved. All other defect types do not preserve stoichiometry.

c) Ti is an element that can exhibit 2+, 3+ and 4+ valence states. Knowing this, is it possible for SrTiO₃ to be nonstoichiometric but remain electrically neutral without the presence of an impurity (something not Sr, Ti or O)? Explain. (2 pts)

Yes. We can imagine a scenario where Ti is in its 2+ state, and we introduce an oxygen vacancy to compensate for the additional 2- charge. We lose stoichiometry, but preserve electronic neutrality without introducing an impurity.

d) Suppose that Gd is introduced to a sample of SrTiO₃. Assuming that it substitutes onto the Sr lattice points, what are the possible types of point defects that could be present as a result? (2 pts)

Substitution of Gd³⁺ for Sr²⁺ results in one additional positive charge. The preservation of charge neutrality will result in either cation vacancies, or anion interstitials.

e) Suppose that for the sample above, the formation energies for Frenkel and Schottky defects are measured to be Qₚ=0.8 eV and Qₛ=1.3 eV respectively. Calculate the equilibrium number of both Frenkel and Schottky defects per cubic meter at T=300K. Hint: recall that you calculated the theoretical density for SrTiO₃ in HW#2. Adapt the expression you used for the density in order to determine N, the total number of lattice sites per cubic meter. (6 pts)

The density calculated for SrTiO₃ in HW#2 was 5.11 g cm⁻³. We can adapt equation 12.1 from Callister to give us the total number of lattice sites per cubic meter as follows:

\[ N = \frac{(n'/V)}{(3A_{O}+A_{Sr}+A_{Ti})} \]
\[ N = \frac{(6.023 \times 10^{23}/\text{mol})(5.11 \text{ g cm}^{-3})(10^6 \text{ cm}^{-3} \text{ m}^{-3})}{(87.62+16*3+47.867 \text{ g/mol})} \]
\[ N = 1.67 \times 10^{28} \text{ lattice sites m}^{-3} \]

We then use equations 12.2 and 12.3 to calculate the equilibrium number of defects.

\[ N_{p} = N \times \exp \left( \frac{Q_{p}}{2kT} \right) = (1.67 \times 10^{28}) \times \exp \left( -0.8 \text{ eV} / (2 \times 300 \text{ K} \times 8.617 \times 10^{-5} \text{ eV K}^{-1}) \right) \]
\[ N_{p} = (1.67 \times 10^{28}) \times (1.905 \times 10^{-7}) = 3.18 \times 10^{21} \text{ defects m}^{-3} \]

&

\[ N_{s} = N \times \exp \left( \frac{Q_{s}}{2kT} \right) = (1.67 \times 10^{28}) \times \exp \left( -1.3 \text{ eV} / (2 \times 300 \text{ K} \times 8.617 \times 10^{-5} \text{ eV K}^{-1}) \right) \]
\[ N_{s} = (1.67 \times 10^{28}) \times (1.2 \times 10^{-11}) = 2 \times 10^{17} \text{ defects m}^{-3} \]
3. **Equilibrium concentration of point defects.**
The energy of formation for a gold (Au) vacancy is approximately ~1.00 eV. Your significant other just bought you a gold ring that he/she claims to be “perfectly crystalline gold”, but you know better and decide to prove him/her wrong.

a) You weigh the ring and discover that it is about 1 gram. Given that gold weighs 197 grams per mole, calculate the total number of atomic sites (gold atoms) in this ring. (6 pts)

\[
\frac{1 \text{ gram}}{(197 \text{ grams/mole})} = 0.00507 \text{ mol} \\
0.00507 \text{ mol} \times 6.02214 \times 10^{23} \text{ atoms/mol} = 3.0569 \times 10^{21} \text{ atoms}
\]

b) Today is an unusually hot day, and the temperature is about 27 °C. Assuming that the ring is at thermal equilibrium with the environment, calculate the total number of vacancies (N_v) in the ring at the current temperature. Boltzmann’s constant is 8.62 \times 10^{-5} \text{ eV/(atom*Kelvin)}, make sure to write out your units. (6 pts)

\[
27+273 = 300 \text{ Kelvin} \rightarrow K_b * 300 \text{ Kelvin} = 0.02586 \text{ eV/atom} \\
N_v = 3.0569 \times 10^{21} \text{ atoms} \times \left[ \exp\left(\frac{-1 \text{ eV}/0.0286 \text{ eV}}{1.6067 \times 10^{17}} \right) \right] = 49115.4 \text{ vacancies}
\]

c) You are furious at being cheated out of N_v gold atoms upon finishing the previous calculation. Your significant other tries to appease you by stating “there are probably an equal number of interstitial atoms as vacancies, so they cancel out.” You check Wikipedia and find the following plot on interstitial concentration in gold. Assuming the data in Wikipedia is accurate, estimate the activation energy from the plot below, and compare with that of vacancies. Is your significant other right, or is he/she lying to you again? (8 pts; 4pts for getting the slope/activation energy right and 4 for explaining that your significant other is wrong.)

*The slope of this line is -10 eV. Since the activation energy of an interstitial is so much higher than a vacancy, it cannot be true that there are equal amounts of both at the same temperature.*
4. Alloys

a) You are designing an intermetallic compound of Al/Ti, which is to be used as a high-strength, low-corrosion, light-weight coating material for an aircraft. The desired material has a final density of 4.08 g/cm$^3$. What weight percent of each component do you need in your alloy in order to achieve this? What is the stoichiometric chemical formula of this intermetallic compound? (8 pts)

The density and atomic weight of Al is 2.71 g/cm$^3$ and 26.98 g/mol respectively and the density and atomic weight of Ti of 4.51 g/cm$^3$ and 47.87 g/mol respectively.

Starting with Eqn 4.10a, $\rho_{\text{avg}} = \frac{100}{C_{\text{Al}} + C_{\text{Ti}}} \rho_{\text{Al}} = \frac{100}{100 - C_{\text{Al}}} \rho_{\text{Ti}}$, rearrange to solve for $C_{\text{Al}}$.

$C_{\text{Al}} = 16\text{wt}\%, \ C_{\text{Ti}} = 84\text{wt}\%$.

Then use Eqn 4.6a&b, $C_1' = \frac{c_4 A_1}{c_1 A_1 + c_2 A_2}$ to determine the atomic%.

$C_{\text{Al}}' = 25\text{at}\%$, $C_{\text{Ti}}' = 75\text{at}\%$.

This indicates a ratio of 3Ti to 1Al atom, so a chemical formula of Ti$_3$Al.
b) You are given a hypothetical alloy that you are told is composed of 20 wt% of metal A and 80 wt% of metal B, which both have the same crystal structure. The density and atomic weight for metal A are 2.55g/cm³ and 18.60g/mol, and for B are 6.43g/cm³ and 39.4g/mol. Determine whether the crystal structure will be simple cubic, body-centered cubic or face-centered cubic, given a unit cell edge length of 0.278 nm. (8 pts)

Starting with Eqn. 3.5,

\[ \rho_{avg} = \frac{nA_{avg}}{V_{cell}N_A} = \frac{nA_{avg}}{a^3N_A} \]

Plug in expressions for \( \rho_{avg} \) and \( A_{avg} \) from eqns 4.10a and 4.11a. Rearrange and solve for \( n \).

\[ n = \frac{100}{\frac{\rho_B}{\rho_A} \frac{a^3N_A}{V_{cell}}} \]

Plug in and find, \( n = 2 \), so body-centered cubic, which has two atoms per unit cell.

c) Describe both an edge and screw dislocation and how they distort the crystal lattice. Include sketches of both and clearly label the burgers vector in each sketch. (4 pts)

An edge dislocation occurs when there is an extra-half plane of atoms that terminates within the crystal. It is a linear defect that centers on the line that is defined along the end of the extra half-plane of atoms. There is local distortion due to the edge dislocation, as atoms above the dislocation (in the figure on the left below) are squeezed together, while the atoms below are pulled apart. The Burgers vector is perpendicular to the edge dislocation.

A screw dislocation can be thought of as being produced by a shear stress, so that one plane, the upper portion (in the figure on the right below) is shifted one atomic distance to the right relative to the bottom portion. The Burgers vector is parallel to the direction of the dislocation.
5. Quartz vs. Glass

a) When examining Quartz(Silica) and Silica Glasses, what is the basic structural unit used to characterize these structures? (3 pts)

When describing the structure of all silica and silica glasses it is convenient to use a basic unit of SiO$_4^{4-}$ tetrahedra.

b) What type of solid (crystalline or amorphous) has a systematic and regular arrangement of atoms over large atomic distances? Which type has a high degree of atomic randomness? (1 pt)

Crystalline solids have a regular arrangement of atoms over large atomic distances. Amorphous solids have a high degree of atomic randomness.

c) Which type of solid has a structure that resembles the atomic arrangement of a liquid? (1 pt)

An amorphous solid has a structure that resembles the atomic arrangement of a liquid. This does not imply the properties of a liquid, but the randomness in its structure is similar to that of a liquid.

d) What type of solid is glass? What type of solid is quartz? (2 pts)

Glass is an amorphous solid.
Quartz is a crystalline solid.

e) Would you expect glass or quartz to form from rapidly cooling an SiO$_2$ melt through its freezing temperature? (2 pts)

When rapidly cooling a melt past the materials freezing temperature, the resulting solid will have a random atomic arrangement similar to that of the liquid. Due to the rapid cooling, there isn’t enough time for the molecules/atoms to form an ordered arrangement. Therefore, glass would be the expected product of cooling an SiO2 melt through its freezing point.

f) Name the three primary polymorphic crystalline forms of SiO$_2$. How many oxygen atoms are shared between SiO$_4^{4-}$ tetrahedra in crystalline SiO$_2$ (This is common to all three polymorphs)? (3 pts)

Quartz, cristobalite and tridymite are all forms of crystalline SiO$_2$ with different arrangements of the SiO$_4^{4-}$ tetrahedra. All four Oxygen atoms of the tetrahedron are shared with neighboring tetrahedra.

g) Additive oxides such as Na$_2$O and CaO are commonly added to silica glasses. What practical effect does the incorporation of the cations of these network modifying oxides have on the melting temperature of the glass? Does the incorporation of these network modifiers make it harder to form the glass at low temperature? (2 pts)
The incorporation of these additives lowers the melting temperature of the glass. The incorporation of these additives does not make it harder to form the glass at low temperature; they make it easier.

h) “Crystal” wine glasses and other glassware were once made of “lead glass” (a silicate glass containing PbO). Treating this “lead glass” as a solid solution of SiO₂ and PbO, find the molar percent concentration of SiO₂ in lead glass containing 30 weight percent PbO. [Hint: molar percent concentration is the molecular form of atomic percent concentration. Treat as molecules and not individual elements (i.e. \(m_{\text{SiO}_2}=m_{\text{Si}}+2m_{\text{O}}\) and 1 mol SiO₂ is \(6.022\times10^{23}\) molecules of SiO₂).] (6 pts)

If the wt% of PbO is 30% then the wt% of SiO₂ is 70%. We can use equation 4.6a from the text to convert from weight percent to molar (atomic) percent.

\[
A_{\text{SiO}_2} = A_{\text{Si}} + 2A_{\text{O}} = 28.09 \text{ g/mol} + 2\cdot16.00 \text{ g/mol} = 60.09 \text{ g/mol}
\]

\[
A_{\text{PbO}} = A_{\text{Pb}} + A_{\text{O}} = 207.2 \text{ g/mol} + 16.00 \text{ g/mol} = 223.2 \text{ g/mol}
\]

\[
C'_{\text{SiO}_2} = \frac{C_{\text{SiO}_2} \cdot A_{\text{PbO}}}{C_{\text{SiO}_2} \cdot A_{\text{PbO}} + C_{\text{PbO}} \cdot A_{\text{SiO}_2}} \cdot 100\% = \frac{70\% \cdot 223.2 \text{ g/mol}}{(70\% \cdot 223.2 \text{ g/mol}) + (30\% \cdot 60.09 \text{ g/mol})} \cdot 100\%
\]

\[
C'_{\text{SiO}_2} = 89.7\%
\]

In other words, in one mole of “lead glass” composed of 70% SiO₂ and 30% PbO by weight there is 0.897 mol SiO₂ and (1-0.897)=0.103 mol PbO. This could be represented by the non-normalized chemical formula: \((\text{SiO}_2)_{0.897}(\text{PbO})_{0.103}\). Which is roughly \((\text{SiO}_2)_9\text{PbO}\) or \(9\text{Si}_9\text{PbO}_{19}\).