UNIVERSITY OF CALIFORNIA
College of Engineering
Department of Materials Science & Engineering

Professor R. Gronsky — Fall Semester 2010

Engineering 45

Midterm 01

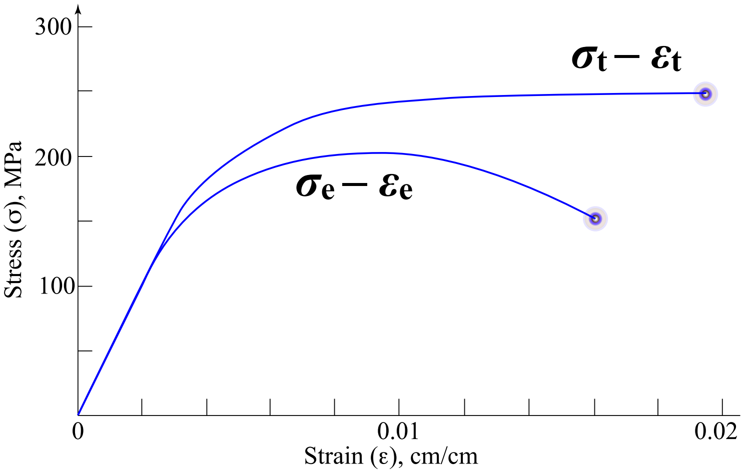
Solutions

INSTRUCTIONS

PATIENCE	Do not open pages until "START" is announced.
PRUDENCE	Position yourself with *occupied* seats directly in front of you and *vacant* seats to your left / right, when possible, unless instructed by exam proctors.
PROTOCOL	Only *writing instruments / eraser / straightedge* are allowed. Remove all other materials, including books / reference materials / calculators / PDAs / cell phones (disable all sounds) / other electronic devices / headphones / ear buds / hats from your person / workplace.
POLITENESS	Asking and answering questions during the exam are very disruptive and discourteous to your classmates. So there will be *no questions* during the exam. Instead, please include your concerns or alternative interpretations in your written answers.
PROFESSIONALISM	The engineering profession demands strict ethical standards of honesty and integrity. Engineers do not cheat on the job, and there will be no cheating on this exam.

1. Mechanical Properties

The stress-strain plots at right are obtained from a single uniaxial tensile test, by varying load (P) and measuring elongation ($\Delta l = l - l_0$) of a test sample before converting to this format. One curve results from a conversion to engineering stress $\sigma_e = P/A_0$ and engineering strain $\varepsilon_e = \Delta l/l_0$, the other, true stress $\sigma_t = P/A_i$ and true strain $\varepsilon_t = \Delta l/l_i$ where the subscripts 0 and i refer to "original" and "instantaneous" values of cross-sectional area (A) and length (l).



a. **Label** the curves as $\sigma_e - \varepsilon_e$ and $\sigma_t - \varepsilon_t$ and **explain the differences** in their appearances.

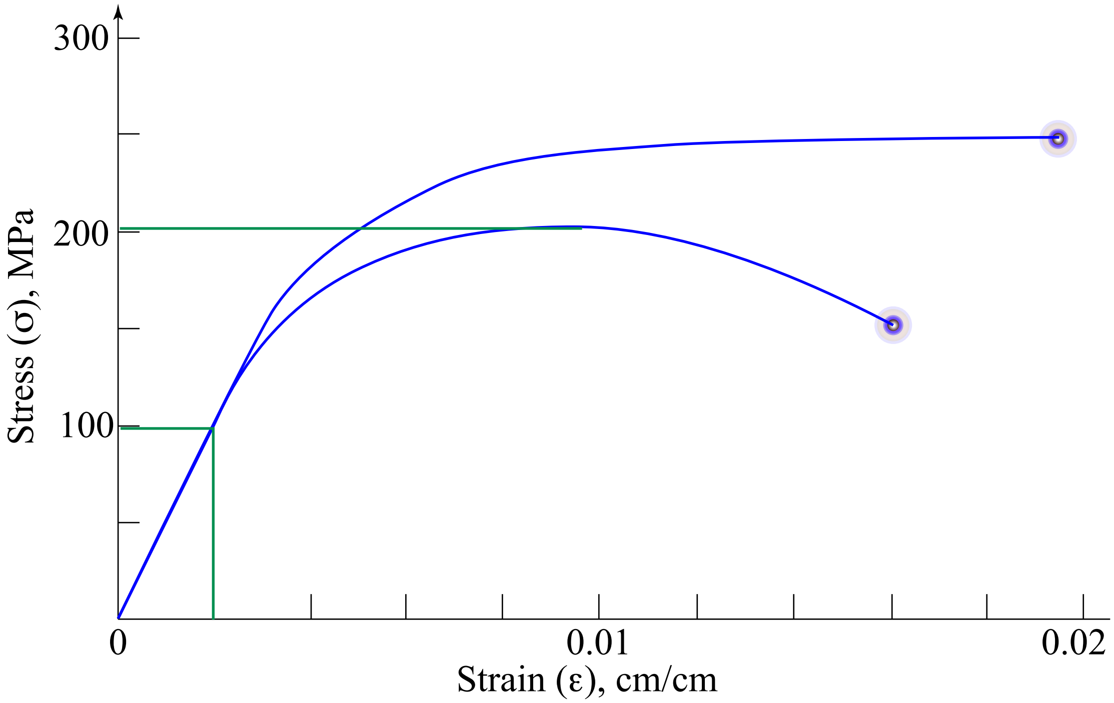
(See **labels** superimposed on figure above). The $\sigma_e - \varepsilon_e$ curve exhibits an inflection point when the cross-sectional area of the sample begins to decrease ("necking"). This decrease is **not** taken into account in the definition of engineering stress, which assumes a constant (original) area. By contrast, there can be no inflection point in the $\sigma_t - \varepsilon_t$ curve because each increment of area reduction is included in the definition.

Both true stress (load divided by instantaneous cross-sectional area) and true strain (change in length divided by instantaneous length) **add incrementally** as deformation proceeds. Both increase monotonically, as exhibited by the shape of the $\sigma_t - \varepsilon_t$ curve.

b. The uniaxial tensile test is conducted according to ASTM standards using a *constant crosshead speed*. **Explain** the significance of this requirement and how it influences the curves shown above.

The requirement of constant crosshead speed is achieved by **reducing the load as necking begins,** which influences the appearance of the $\sigma_e - \varepsilon_e$ curve. It is the **reason for the inflection point**. It's significance is that it enables an **identification of the onset of necking**, and the definition of the **ultimate tensile strength**, both of which are pinned to the inflection point in the $\sigma_e - \varepsilon_e$ curve. Without the ASTM standard, these terms would have nebulous meaning.

1. Mechanical Properties



c. What **value** would you specify as the **elastic modulus** of this alloy? **Explain**.

The "elastic" modulus, also known as "Young's Modulus" (E) is the slope of the initial portion of the stress-strain curve where Hooke's Law applies.

$$\sigma = E\varepsilon$$

Both $\sigma_e - \varepsilon_e$ and $\sigma_t - \varepsilon_t$ curves share this linear behavior, which is due to the stretching of atomic bonds, before any bond-breaking commences. It can be calculated directly from the plot, using convenient values such as the following

$$E = \frac{\Delta\sigma}{\Delta\varepsilon} = \frac{[100 - 0]\ \mathrm{MPa}}{[0.002 - 0]\ \mathrm{cm/cm}} = \mathbf{50}\ \mathrm{GPa}$$

d. What **value** would you specify for the **ultimate tensile strength** of the alloy? **Explain**.

This is read directly from the $\sigma_e - \varepsilon_e$ curve. It is the "peak" value at the inflection point, shown on the figure above to be **UTS = 200 MPa**.

2. Bonding

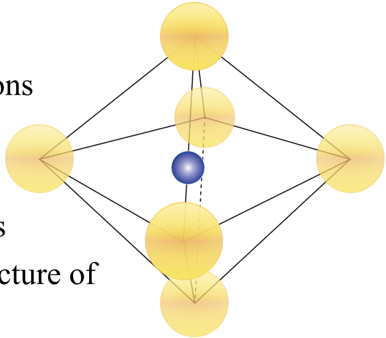
a. Simeon-Denis Poisson was a French mathematician who related elastic strain normal to the stress axis (ε_x) to elastic strain along the stress axis (ε_z) as a ratio, which now bears his name (Poisson's ratio), and is written as

$$\nu = -\frac{\varepsilon_x}{\varepsilon_z}$$

Type 304 stainless steel is a high strength metallic alloy with an fcc structure and $\upsilon = 0.29$, while aluminum bronze is a lower strength metallic alloy with an fcc structure and $\upsilon = 0.33$.
Explain, citing concepts of metallic bonding.

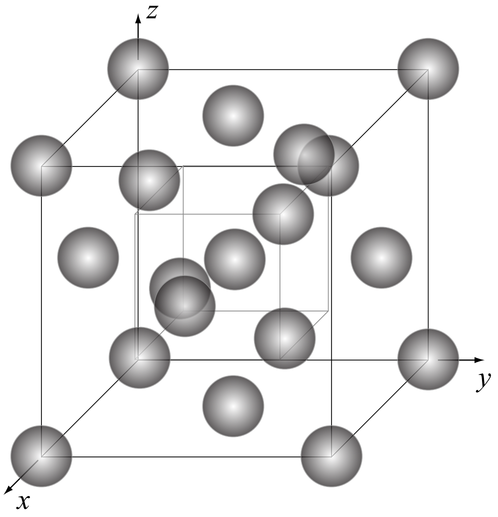
Metallic bonds result from the delocalization of the valence electrons that participate in bonding, enabling global "sharing" of those electrons among many ion cores, generating bonds that are "non-directional." The observed differences in Poisson's ratio between two "metallically bonded" solids (steel and bronze both exhibit the properties expected of "metals") suggests that this is not always the case, and some directionality may be at play. Under these circumstances, the accepted explanation is an intrusion of some "covalent character" to the bonds, as also used to rationalize the CN=8 in BCC metals, for example.

b. Alumina (Al_2O_3) is an oxide ceramic formed from trivalent aluminum cations and divalent oxygen anions. The radius ratio of cation to anion (r/R) in alumina is 0.4318, in the range $0.414 \leq r/R \leq 0.732$, associated with a coordination number of 6. **Explain** how the nature of ionic bonding causes the coordination number to be a prominent consideration in the crystal structure of oxide ceramics.



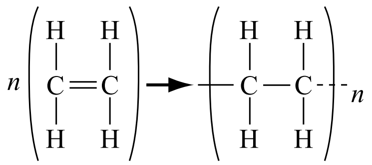
Ionic bonding is the result of "charge transfer," which creates two oppositely charged ions that succumb to the influence of Coulombic forces to establish a "bond" at equilibrium (zero force condition). Such a bond is "non-directional" suggesting that bonding can occur in *any* direction. However, during charge transfer, cations decrease in size, and anions increase in size, imposing a size effect on how they can pack together in the solid state. This packing geometry is limited by the radius ratio, and the resulting coordination number, influencing the development of crystal structure in ionic solids.

2. Bonding



c. When $r = R$ (not possible in ionic solids), the radius ratio cited in (**b**) above is $r/R = 1$, and the coordination number is 12, as found in such metallic crystals as Al, Cu, Ni, Ti, and many others. However, when carbon atoms bond to other carbon atoms ($r = R$) forming diamond, the coordination number is 4. **Explain**, citing concepts of covalent bonding.

Covalent bonding is described as the "mutual" sharing of electrons, facilitated by the overlap of valence electron orbitals. Unlike metallic bonding, in which those orbitals are fully delocalized, covalent bonding results from **localized** orbital overlap, rendering the bonds "directional." The bonds form along directions of **greatest orbital overlap**. In the case of diamond, carbon bonds covalently after sp_3 hybridization, which limits the number of C bonds that can be formed by localized orbital overlap to 4, resulting in CN = 4, and the "diamond cubic" crystal structure shown in the figure.



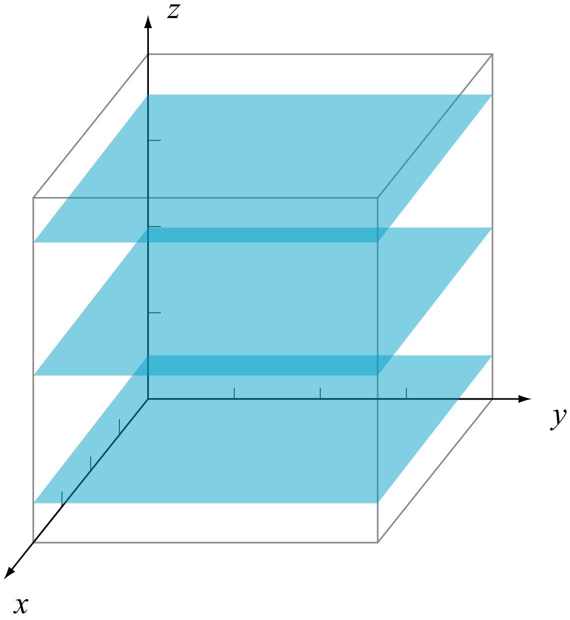
$$n\left(\mathrm{H_2C{=}CH_2}\right) \longrightarrow \left(\mathrm{-CH_2-CH_2-}\right)_n$$

d. Carbon-carbon bonds in polyethylene are also covalent, yet polyethylene softens at 120°C while diamond softens (melts) at 3500°C. **Explain**.

Polyethylene is a polymer with a backbone chain of covalently-bonded carbon atoms, but the chains are bonded to one another by electrostatic dipole interactions. Such dipole interactions are induced by the large groups of atoms on adjacent backbone chains, which generate weak bonds, called "secondary" bonds, to distinguish them from "primary" bonds that form between individual atoms or ions. In diamond, ALL bonds between all carbon atoms are primary (covalent) bonds, resulting in a much stronger material, as the difference in "softening" temperatures between these two materials confirms.

3. Lattice Geometry

a. Identify the family to which the following planes in a cubic lattice belong. Use Miller index notation.

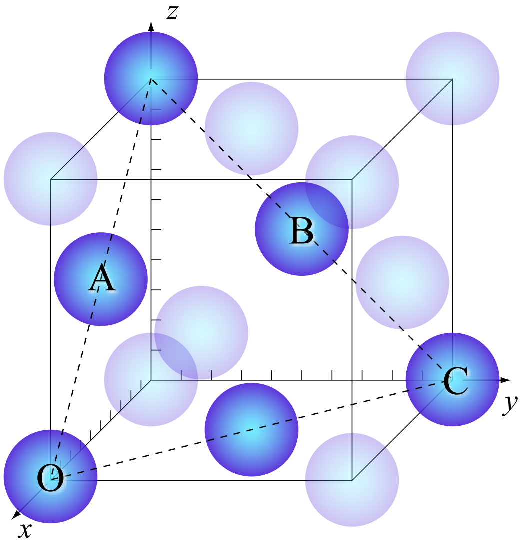


Referring to the plane closest to the origin in this figure, its intercepts with the coordinate axes are ∞, ∞, ⅛. Taking the reciprocals, clearing fractions (unnecessary here) and enclosing in parentheses, the answer is

$$(008)$$

Check: the other planes are parallel to this one, and appear at intersections ½ and ⅞ along the *z* axis, confirming that they belong to the same (008) family.

b. The figure below shows one member of the (111) family of planes in a face-centered cubic structure. Specify in Miller index notation the lattice directions connecting the following pairs of atoms.



$$\overrightarrow{OA} = [\bar{1}01]$$

$$\overrightarrow{OB} = [\bar{2}11]$$

$$\overrightarrow{OC} = [\bar{1}10]$$

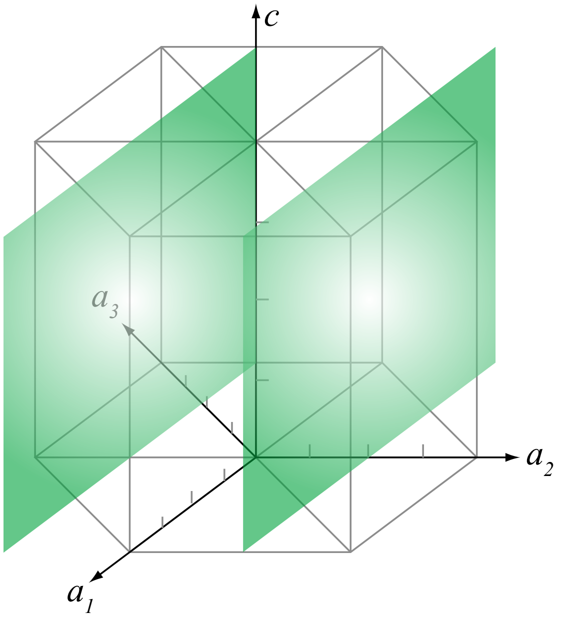
$$\overrightarrow{AB} = [\bar{1}10]$$

$$\overrightarrow{AC} = [\bar{1}2\bar{1}]$$

Check: **Dot product = 0** for all directions in the (111) plane with [111] normal.

3. Lattice Geometry

c. Specify in Miller-Bravais notation the family of planes containing the following planes as members.

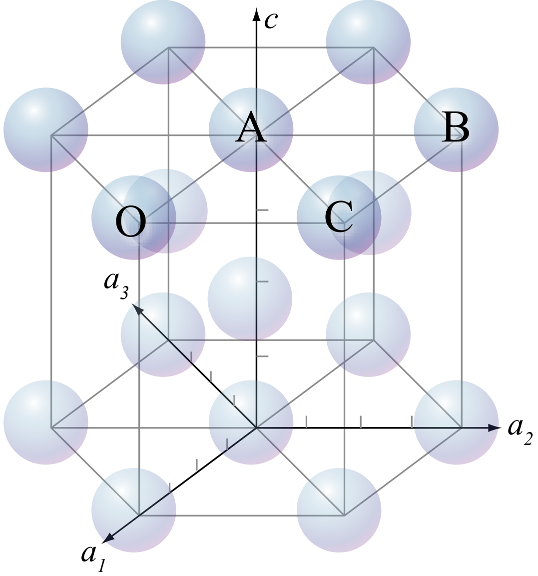


Referring to the plane to the right of the origin in this figure, its intercepts with the coordinate axes are ∞, ½, –½, ∞. Taking the reciprocals, clearing fractions (unnecessary here) and enclosing in parentheses, the answer is

$$(02\bar{2}0)$$

Check: the parallel plane to the left of the origin has intercepts ∞, –½, ½, ∞, confirming that it belongs to the same family.

d. The figure below shows one member of the (0001) family of planes in an hexagonal close-packed structure. Specify in Miller-Bravais index notation the lattice directions connecting the following pairs of atoms.



$$\overrightarrow{OA} = [\bar{2}110]$$

$$\overrightarrow{OB} = [\bar{1}100]$$

$$\overrightarrow{OC} = [\bar{1}2\bar{1}0]$$

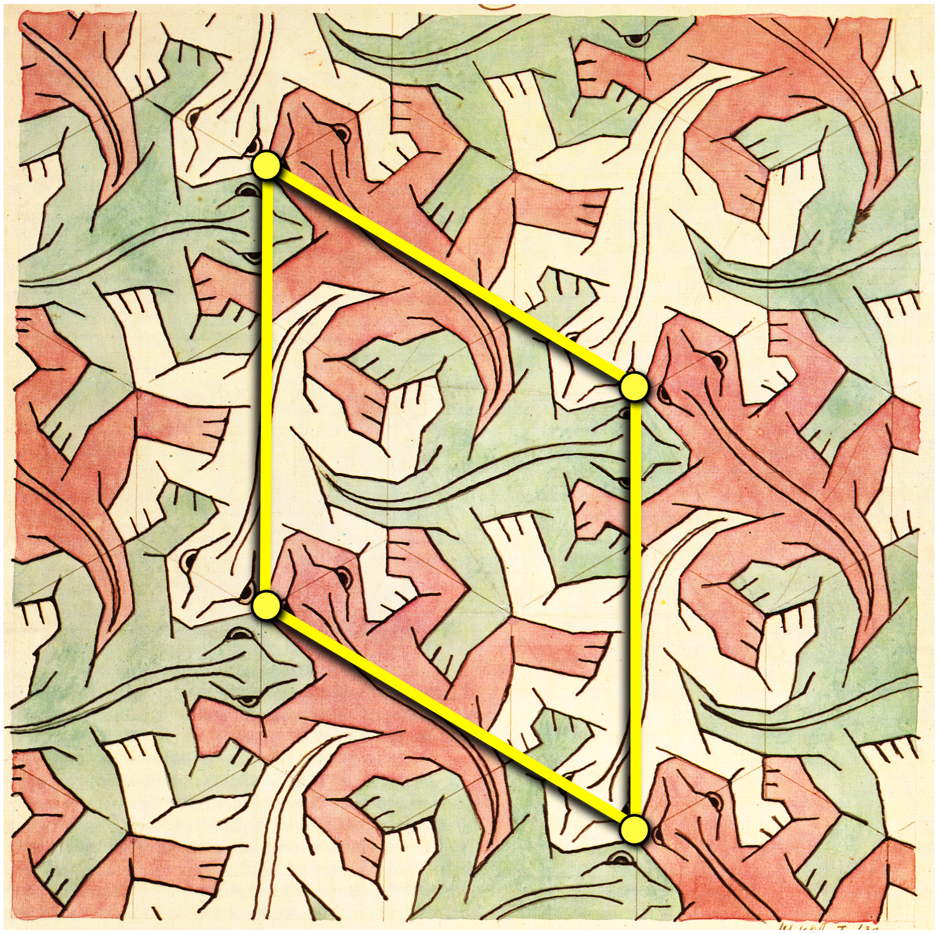
$$\overrightarrow{AB} = [\bar{1}2\bar{1}0]$$

$$\overrightarrow{AC} = [11\bar{2}0]$$

Check: $h + k = -i$

4. Crystal Structure

a. Refer to the following drawing[1] by M.C. Escher entitled "Study of Regular Division of the Plane with Reptiles" produced with pencil, India ink and watercolor in 1939. Show directly on this drawing the points of a **lattice**, and a **primitive unit cell** that fully describes the "structure" of the periodic image.



b. Recall that a periodic (for example, "crystal") structure can be described by the combination of a lattice and a "motif" that must be assigned to each and every lattice point in the same orientation. Now specify the "**motif**" associated with the periodic structure of this Escher image.

Both the motif and the unit cell must fully describe the "crystal." The motif can be therefore discerned from the contents of the unit cell: the unit cell contains 3 reptiles, so must the motif. The **motif** above is: **1 yellow reptile, 1 red reptile and 1 green reptile** arrayed in clockwise fashion in the same fixed orientation shown at each lattice point.

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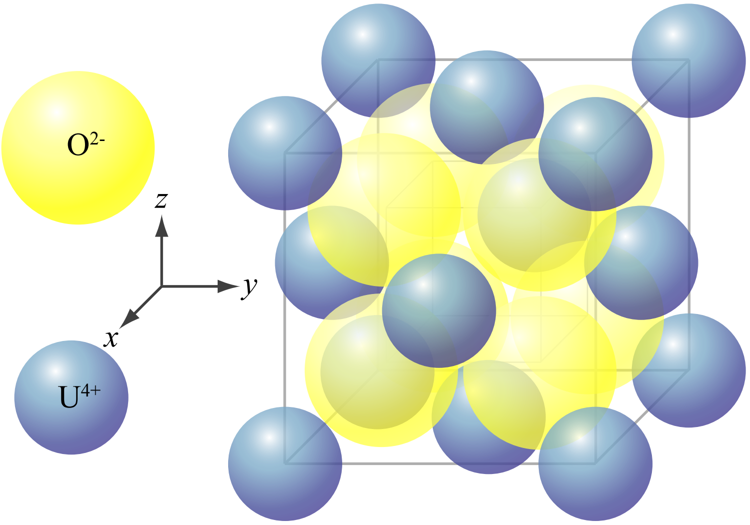
[1] *The World of M.C. Escher*, J.L. Locher, (Ed.), H.N. Abrams, Inc. Publisher, New York (1971).

4. Crystal Structure

c. The cubic unit cell describing one of the oxides of uranium used as a fuel in nuclear reactors has uranium cations at locations 0,0,0; 0,½,½; ½,0,½; and ½,½,0, with oxygen anions at ¼,¼,¼; ¼,¾,¼; ¾,¼,¼; ¾,¾,¼; ¼,¼,¾; ¼,¾,¾; ¾,¼,¾; and ¾,¾,¾. Specify the **lattice** and **motif** that defines this structure. What is its **chemical formula**?

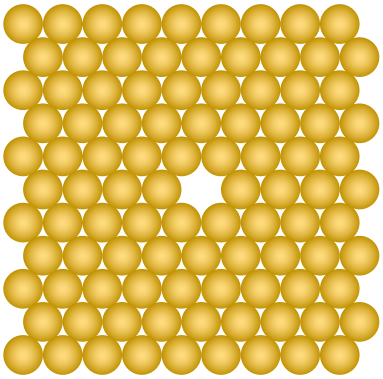


The uranium cations occupy FCC sites and the oxygen anions occupy all of the tetrahedral interstices (the corners of the interior cube indented by ¼ of the lattice constant from all faces). There are 4 uranium ions per unit cell and 8 oxygen ions per unit cell (given); this establishes the stoichiometry of the crystal, 2 oxygens for each uranium, which must also be true of the motif. Consequently, the **lattice is face-centered cubic (FCC)** and the motif must contain at least three ions, 1 uranium and 2 oxygens. There are several options, but the most common one is to site them symmetrically about each lattice point, so an acceptable **motif** is **1 uranium cation at 0,0,0 and 2 oxygen anions, one at +¼,+¼,+¼, and the other at –¼,–¼,–¼**. Finally, the same ratio must be preserved in the **chemical formula:** $\mathbf{UO_2}$. Note the charge on the ions and the need to preserve charge neutrality.

d. In a diffraction experiment designed to utilize Bragg's Law ($n\lambda = 2d \sin\theta$), a single crystal of this nuclear fuel pellet is oriented so an incident beam of Cu $K\alpha$ radiation ($\lambda = 0.154$ nm) makes an angle of 14.22° with the (040) family of planes. At what angle should the detector be positioned to capture the 040 diffraction peak?

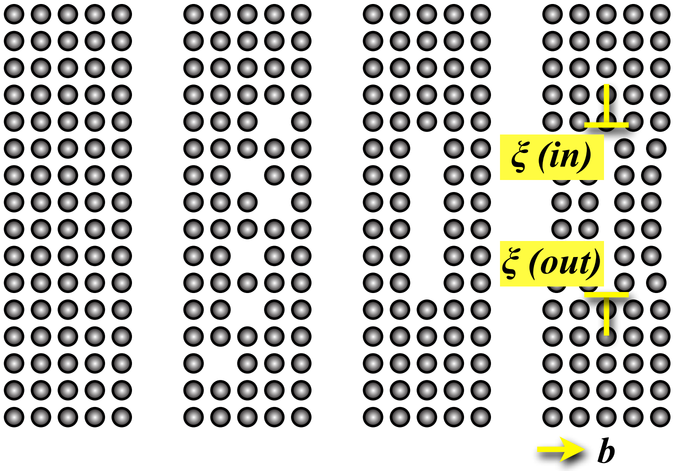
In all Bragg experiments, the scattering condition is established to mimic "reflection" from the diffracting planes, so the incident angle is equal to the diffraction angle. The detector should therefore be positioned at **14.22°** from the sample surface, opposite the source.

5. Crystal Defects



a. It is claimed that vacancies are not true "point" defects (zero-dimensional) because they exert a tensile stress on the atoms surrounding them, extending over finite dimensions. Consider the illustration of a single close-packed plane containing a vacant site shown to the right. Is there a tensile stress in the vicinity of the vacancy or not? **Explain**.

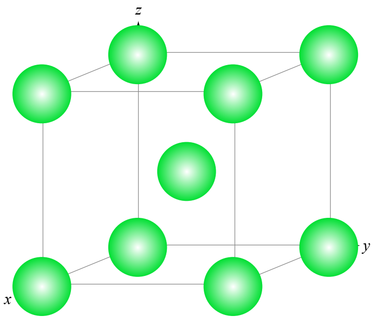
There appears to be no room to "collapse" into the vacant site when all atoms are touching one another in this plane, but the "hard sphere" model is inaccurate here. There is a collapse into the gap by all contiguous atoms, which in turn stretch their bonds to their nearest neighbors, the equivalent response to a tensile load. So the strain field is "tensile."



b. Vacancies are created at high temperatures in concentrations that obey an Arrhenius-type relation. Also at temperatures sufficient to cause diffusion, vacancies can "condense" into dislocation "loops," as shown in an edge-on projection here, with time increasing from left to right. Label both the **line direction vector** (ξ) and the **Burgers vector** (***b***) of the dislocation loop in the final frame. What **type** of dislocation (edge or screw) is it?

The **line direction vector** (ξ) runs both **into** and **out of** the plane of the paper, because it follows the loop, either in at the top, out at the bottom, or the reverse (it may arbitrarily assigned). The **Burgers vector** (***b***) however is fixed by the FSRH convention to **point to the right** with a magnitude of **one interatomic spacing**. Because $\xi \perp b$, the dislocation loop is **pure edge**.

5. Crystal Defects

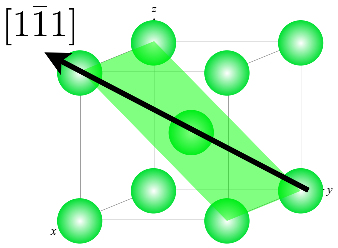


c. In BCC crystals, active slip systems consist of close-packed $< 111 >$ directions and the $\{1\bar{1}0\}$ planes that contain those directions. Consider an edge dislocation with a Burgers vector

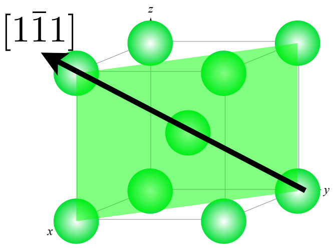
$$\mathbf{b} = \frac{a}{2}[1\bar{1}1]$$

Specify the possible **slip planes** for this edge dislocation.

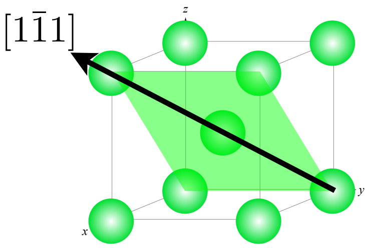
By definition, the slip plane must contain the Burgers vector, and in this instance there are three possible candidate slip planes.



(011)

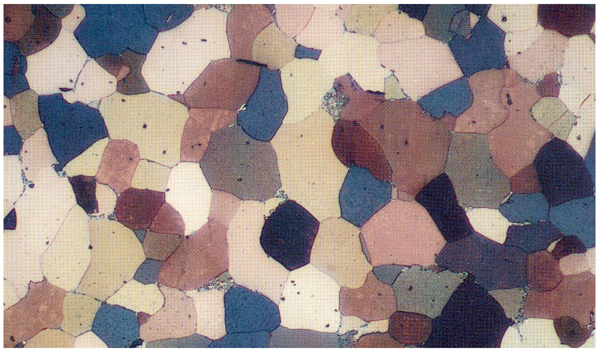


(110)



$(\bar{1}01)$

Check: Dot product between ***b*** and all three plane normals = 0



d. Nearly all engineering materials are polycrystalline, with individual grains meeting at internal interfaces known as grain boundaries to establish a very important characteristic "grain size." A universal tenet of engineering materials is "fine-grained alloys are stronger than coarse-grained alloys." **Explain**.

Strength on a microstructural scale is resistance to the nucleation and migration (slip) of dislocations. Grain boundaries act as barriers to dislocation motion by disrupting the continuity of slip planes; the more grain boundaries appearing in the path of mobile dislocations, the greater the number of impediments to their motion. Consequently, for any engineering alloy, fine grained microstructures with their higher density of grain boundaries resist dislocation motion more coarse grained microstructures. They are "stronger" as a result.