SOLUTIONS

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

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Fall Semester 2014

Engineering 45

Midterm 02

This is a 50 minute examination with 4 equally weighted problems.

Instructions

WAIT! Do not open these pages until "START" is announced.

While you are waiting please
PRINT your name **clearly** and **legibly** at the top of this page,
SILENCE your mobile phones and other electronic devices,
STORE all belongings under your seat and out of sight, and
NOTE the following rules.

ONLY writing instruments / eraser / straightedge are allowed.
Calculators are NOT allowed.
Questions during the exam are NOT allowed.
You ARE held to your Honor Code!

UCLA is coming to town this weekend. GO BEARS!!

Worksheet

(There will be no points awarded for work shown on this page. Enter your answers on the following pages in the space provided.)

Useful Relations

$$n\lambda = 2d_{hkl}\sin\theta$$

$$\text{rate} = Ce^{-Q/RT}$$

$$\frac{\partial C_x}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial C_x}{\partial x}\right) = D\frac{\partial^2 C_x}{\partial x^2}$$

$$D = D_0 e^{-q/kT}$$

$$\overrightarrow{V_1}\cdot\overrightarrow{V_2} = |V_1||V_2|\cos\delta$$

$$d_{hkl} = \frac{a_0}{\sqrt{h^2+k^2+l^2}}$$

$$\frac{n_v}{n_{sites}} = Ce^{-E_v/kT}$$

$$\frac{C_x - C_0}{C_s - C_0} = 1 - \text{erf}\left(\frac{\text{x}}{2\sqrt{\text{Dt}}}\right)$$

“REFLECTION RULES”	Allowed	Forbidden
Simple Cubic	all	none
Body-Centered Cubic	$h+k+l =$ even	$h+k+l =$ odd
Face-Centered Cubic	h,k,l unmixed (even/odd)	h,k,l mixed (even/odd)

Problem	Possible	Score
1	25	
2	25	
3	25	
4	25	
TOTAL	100	

Problem (1)

The “diamond cubic” crystal structure exhibited by the Group IV elements is based on a face-centered-cubic (fcc) Bravais lattice with a two-atom motif, one at 0,0,0 and the other at ¼, ¼, ¼.

(a) Sketch a cube axis projection of the diamond cubic structure labeling the location of all eight atoms contained within a single fcc unit cell.

(b) Sketch on this projection the lattice direction connecting the atom at location 1,0,0 with the atom at the tetrahedrally-coordinated position ¼, ¼, ¼.

(c) What are the indices of this lattice direction?

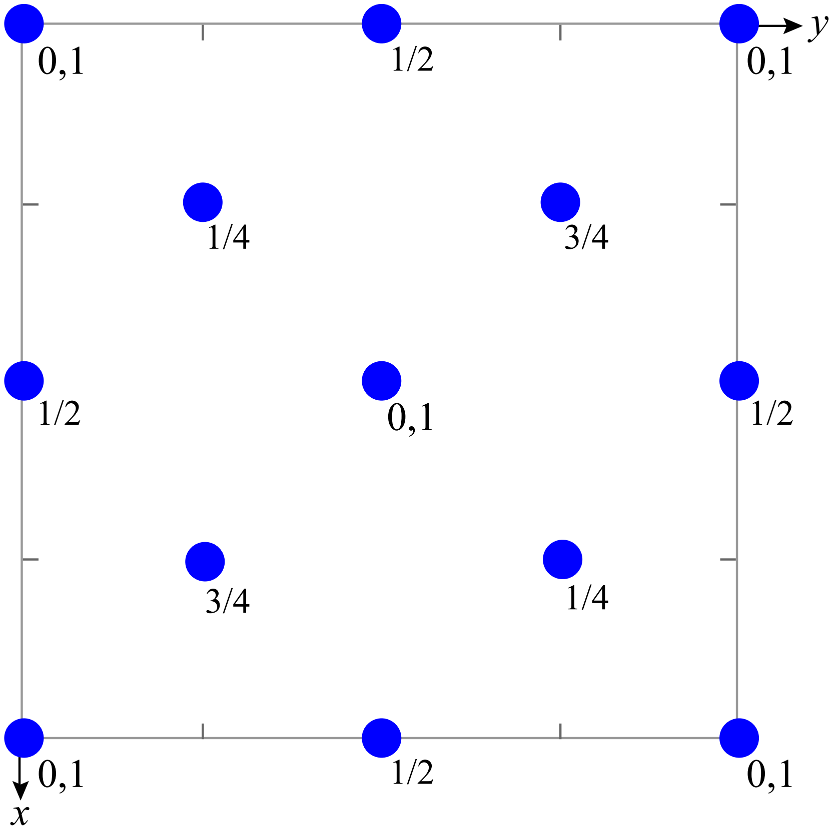
(d) Sketch on this projection within the unit cell all members of the family of planes having the smallest *d*-spacing that contain the lattice direction you’ve just identified.

(e) What are the Miller indices of this family of lattice planes?

Answer (1)

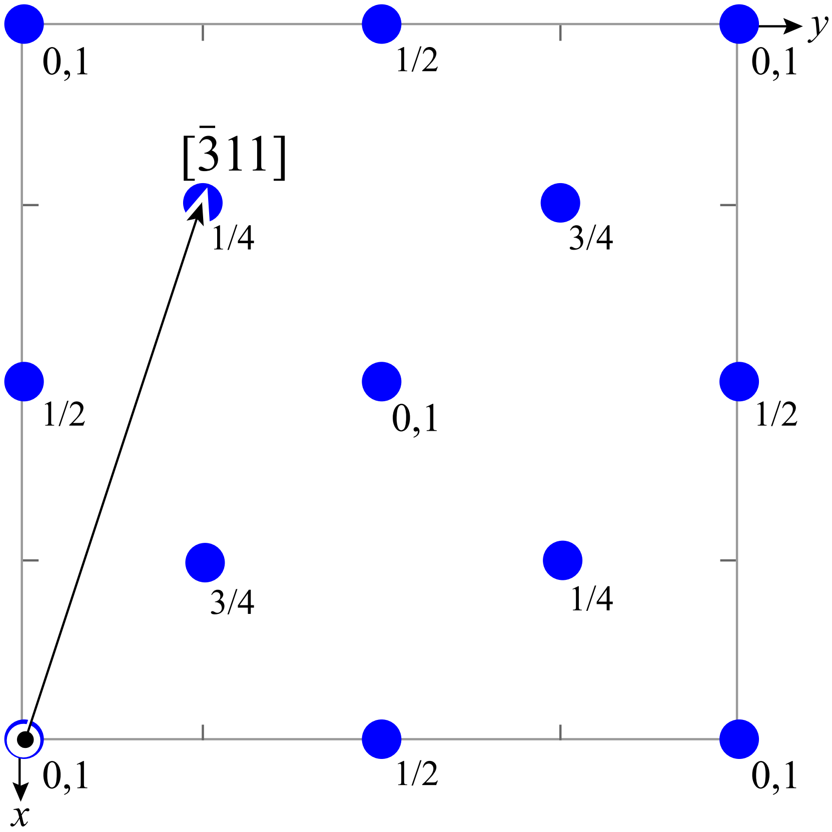
(a) The origin of the lattice is in the upper left hand corner of this figure, by the intersection of the labeled *x* and *y* axes, so all atom positions in the projection of the unit cell shown here are labeled accordingly. The labels indicate the height above the *x*-*y* plane at the origin.

The atoms are found at the corners (8 × 1/8 = 1) plus the face centers (6 × ½ = 3) plus the four occupied tetrahedral interstices (4 × 1 = 4) for a total of eight within this unit cell.



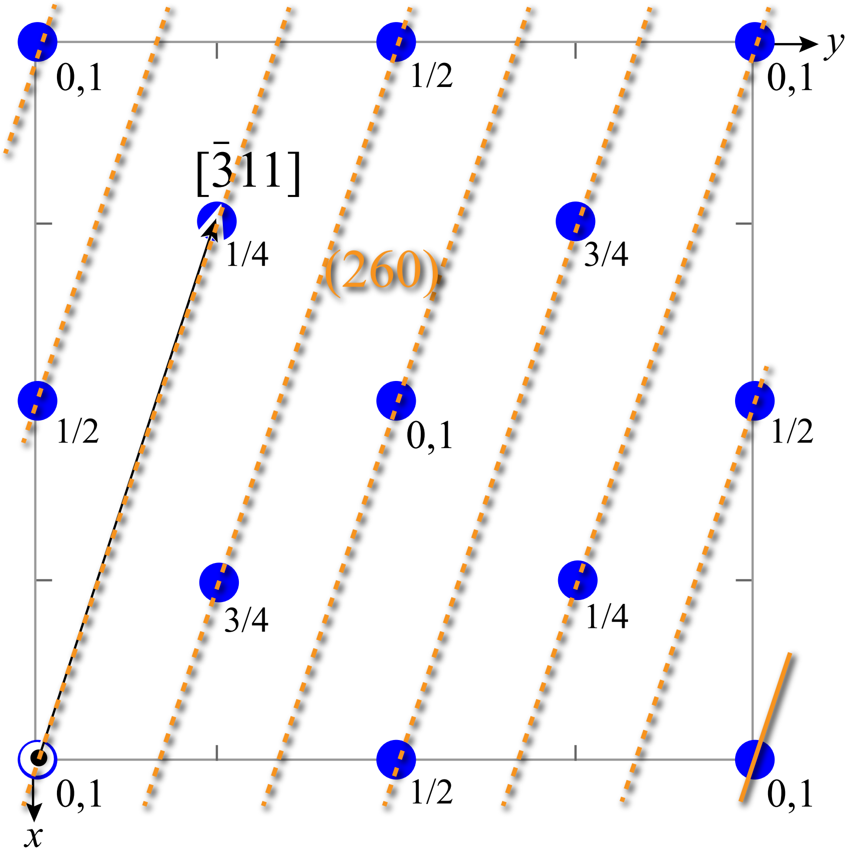
Answer (1) continued

(**b**) The lattice direction connecting the atoms at locations 1,0,0 and ¼, ¼, ¼ is sketched here.



(**c**) Its index is obtained by shifting the origin to 1,0,0 and subtracting from ¼, ¼, ¼ to obtain the new location, –¾, +¼, +¼, relative to the new origin. Clearing fractions yields the lattice direction $[\bar{3}11]$ as shown here. Note that it can also be deduced by traversing –¾ along the *x*-direction, +¼ along the *y* direction, and another +¼ along the *z*-direction from the new origin at 1,0,0, yielding the same index.

(**d**) The family of planes containing the lattice direction above is shown by constructing parallel lines through all of the atom positions and noting the smallest *d*-spacing that results.



(**e**) These are indexed by noting the fractional intercepts, which, from the origin (upper left point) are ½ along the *x*-axis, and 1/6 along the *y* axis, generating the Miller indices (260) as labeled. The normal to these planes is the [260] direction, confirmed by dot product with the $[\bar{3}11]$ direction to be the correct index (dot product is zero).

Problem (2)

The Hospital for Special Surgery (HSS) in New York City requests your assistance as a consultant on a patient injury case caused by the fracture of a "bone saw" during orthopedic surgery. The saw was advertised to the surgeons as having a "perfectly stoichiometric WC coating" to "retain edge sharpness." You request and obtain diffraction analysis from three independent labs of the tungsten carbide powder that was diffusion-bonded to the steel blade. All three confirm the atom positions within a *c*-axis projection of the unit cell illustrated here.

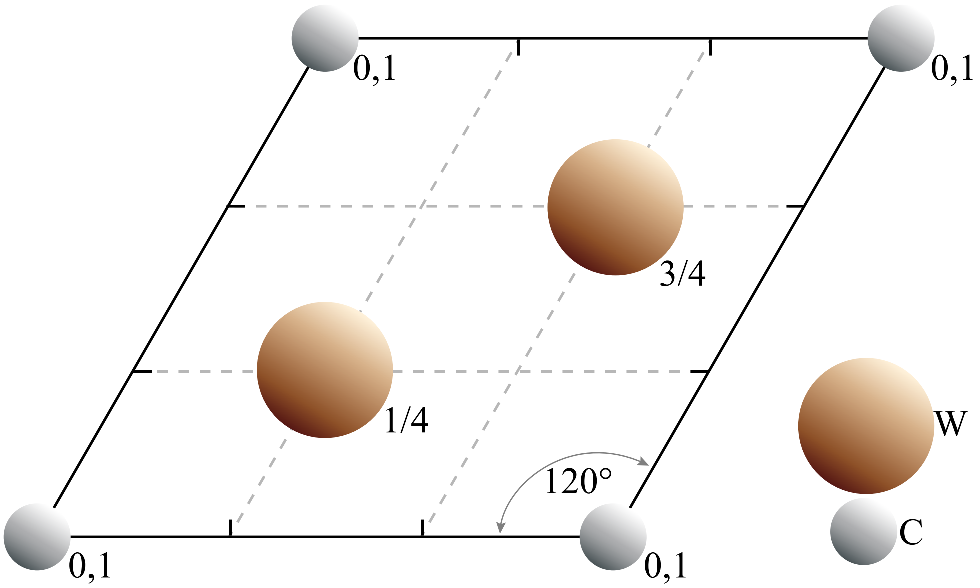
(**a**) What is the Bravais lattice?

(**b**) What is the motif or basis?

(**c**) What are the complete contents of the unit cell?

(**d**) What is the chemical formula of the compound?

(**e**) On the basis of this finding, what do you report to HSS about the cause of the bone saw failure?



Answer (2)

(a) The projection clearly has two equal-length axes in the plane projection with an unknown dimension for the *c*-axis along which the projection is made. An included angle of exactly 120° (the other being 60°) confirms that system is hexagonal, and there is only one Bravais lattice in the hexagonal crystal system, **simple hexagonal.**

(**b**) The simple hexagonal Bravais lattice has lattice points at all locations labeled 0,1 on this projection, which are the corners of the unit cell. The motif must be associated with each and every lattice point, requiring a **three-atom** assignment, **one C atom at 0,0,0, one W atom at ⅔, ⅓, ¼, and one W atom at ⅓, ⅔, ¾**.

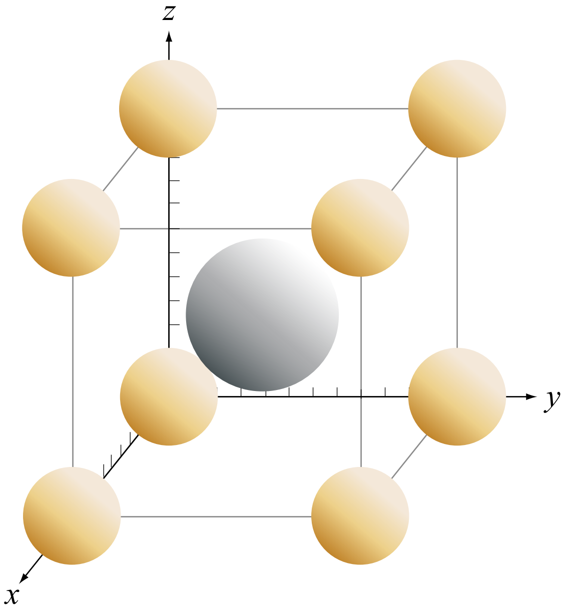
(**c**) A simple hexagonal unit cell is primitive, so it contains a single lattice point. From (**c**) above, every lattice point contains one C atom and two W atoms. Consequently the complete contents of the unit cell must be **one C atom and two W atoms**. These can also be "counted" from the projection: one C atom is shared by all corners with adjacent cell, and two W atoms are fully contained within the cell.

Answer (2) continued

(**d**) Both the motif and the contents of the unit cell must preserve the stoichiometric balance of the compound, expressed as a minimum. In this case they are all the same, and the formula is **W_2C**.

(**e**) Your ethical mandate is to report to the HSS that you **do not know the cause** of the bone saw failure. You can of course report that you made an interesting discovery that the coating is a di-tungsten carbide, W_2C, and NOT the stoichiometric tungsten carbide, WC, that it is advertised to be. But you have **not** established any link to failure.

Problem (3)

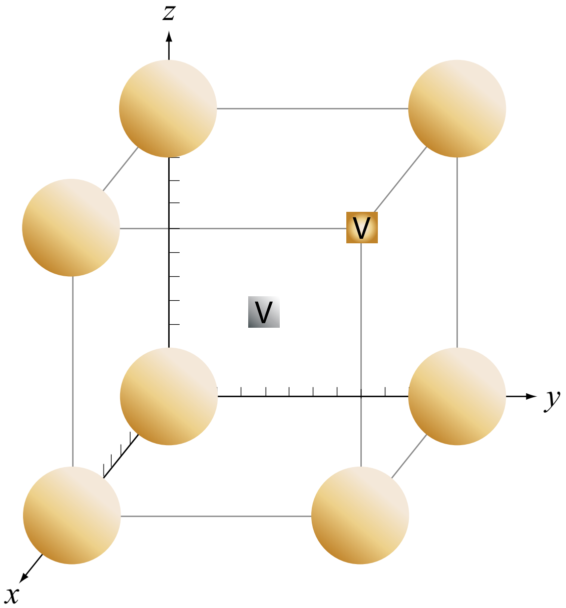


Cesium chloride adopts a cubic crystal structure as illustrated here. Consider the defects of different dimensionality that might be present in such a compound.

(**a**) According to Wikipedia[1], "A defect in which an atom, such as silicon, is missing from one of the lattice sites is known as a 'vacancy' defect. It is also known as a Schottky defect, although in ionic crystals the concepts are not identical."
What do you say? Use cesium chloride to illustrate your reasoning.

(**b**) How many slip systems are there in cesium chloride? Explain, citing their identity.

Answer (3)



(**a**) A vacancy defect is **not** "also known as a Schottky defect." While vacancy defects can be found in silicon, Schottky defects cannot. The reason is that **Schottky defects are a class of point defects that occur ONLY in ionic crystals**. A single vacancy in an ionic crystal would cause a charge imbalance. A Schottky defect is a **pair of vacancies**, **one anion vacancy and one cation vacancy** that are coupled because together they **preserve charge neutrality**. Maybe this is the meaning (?) of that wiki phrase "in ionic crystals the concepts are not identical."

In the case of cesium chloride, the pairing of a Cs^+ vacancy and a Cl^- vacancy constitutes a Schottky defect, as sketched here. While there may appear to be a charge imbalance in a single unit cell, balance is restored when averaged over the entire macroscopic crystal.

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[1] < http://en.wikipedia.org/wiki/Vacancy_defect >

Answer (3) continued

(**b**) For CsCl, the Bravais lattice is simple cubic, populated by a two-ion motif, one Cs^+ at 0,0,0 and one Cl^- at ½, ½, ½. In any crystal system the Burgers vector of a slip dislocation is the shortest lattice translation vector, which in the case of a SC lattice is the cube edge.

Consequently the slip directions are of the **<001> type**.

The slip planes would then be the closest-packed planes containing these slip directions, or the planes of the **{100} type**.

Therefore since there are **3 different families of {100} planes in the simple cubic Bravais lattice, each containing 2 orthogonal <001> directions**, the total number of slip systems in CsCl is 3 × 2 = **6**.

Problem (4)

You are the chief design engineer on a project that requires small electric motors running at 150°C. In preliminary tests at this temperature, the motors fail because the small copper wires in the armature windings oxidize. A member of your engineering staff suggests that you need a “diffusion barrier” on the Cu to protect against oxidation, and suggests Ag, another good conductor. You are concerned that the Ag might diffuse into the Cu at 150°C, reducing its protective quality, so you decide to calculate the thickness of Ag required to maintain surface coverage of the Cu for 5 years. The most accurate data available to you is for Ag diffusion into Cu at temperatures between 750°C and 1050°C. Extrapolating this data to 150°C, you calculate that a 1 µm thick layer of Ag will last 100 years. You then do the experiment, with a 1 µm think layer of Ag deposited onto Cu and heated to 150°C, only to discover that the Ag completely diffuses into the Cu over one weekend!

What went wrong? Why was the calculation of your rate at 150°C invalid? Explain.

Answer (4)

What went wrong was a poor assumption, that all diffusion occurs as “volume” diffusion. You forgot that commercial wires are polycrystalline, full of grain boundaries, and these grain boundaries serve as high-diffusivity paths, especially prominent at low temperatures.

More specifically, your diffusion data for Ag in Cu was obtained at relatively high temperature, when volume diffusion is very fast, fast enough to be competitive with grain boundary diffusion. Extrapolating this data to low temperatures on the assumption that all diffusion occurs “through the bulk,” rather than through defects, rendered a very low calculated diffusion flux. But at low temperatures, grain boundary diffusion can be orders of magnitude faster than volume diffusion, as your experimental measurements illustrated, confirming the fallacy of your assumption.