MSE-2001H September 15th 2015

Name ____(***Please Print Your name***)

Exam-1: Chapters 1-3

Useful equations

$$F \propto \Delta x, \quad \frac{F}{\Delta x} = aE, \quad \frac{\partial^2 U}{\partial x^2} = aE, \quad \frac{x_e - x_0}{x_0} = \alpha(T_e - T_0)$$

BCC: $a_0 = \frac{4r}{\sqrt{3}}$, FCC: $a_0 = \frac{4r}{\sqrt{2}}$, HCP: $a_0 = 2r$, $c = \left(\frac{4}{\sqrt{6}}\right)a_0$

Critical r/R	0~0.155	0.155~0.225	0.225~0.414	0.414~0.732	0.732~1	1
CN	2	3	4	6	8	12

Packing factor = (Number of spheres x vol. of sphere) / vol. of unit cell

$$\rho_L = \frac{\text{Number of atoms centered along direction within one unit cell}}{\text{Length of the line contained within one unit cell}}$$

$$\rho_P = \frac{\text{Number of atoms centered on a plane within one unit cell}}{\text{Area of the plane contained within one unit cell}}$$

$$\text{APF} = \frac{(\text{Number of atoms in cell}) \times (\text{Volume of an atom})}{\text{Volume of the unit cell}}$$

Bragg's law: $m\lambda = 2\, d_{hkl} \sin\theta$

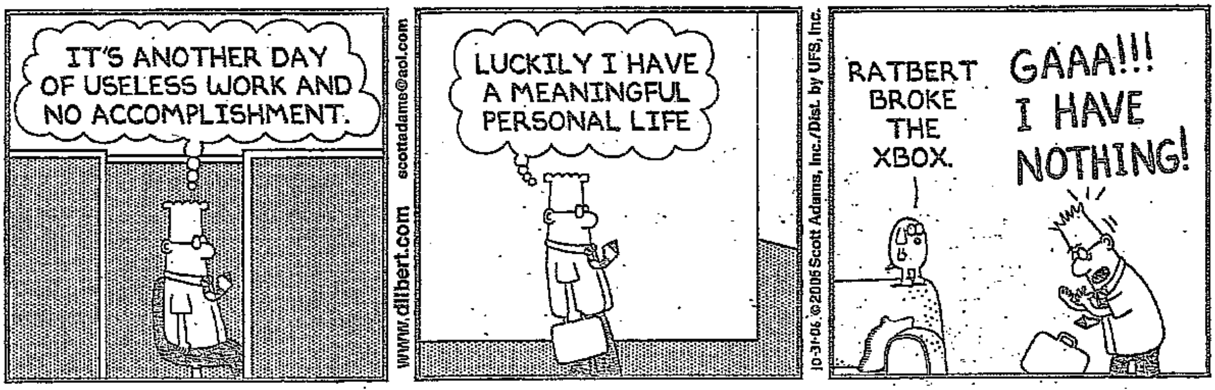
Spacing between the planes: $d_{(hkl)} = \frac{a_o}{(h^2 + k^2 + l^2)^{\frac{1}{2}}}$

Angle between two directions: $\theta = \cos^{-1}\left[\frac{uu' + vv' + ww'}{\left(u^2 + v^2 + w^2\right)^{1/2}\left(u'^2 + v'^2 + w'^2\right)^{1/2}}\right]$

Part	**Points**	**Maximum**
A		**20**
B		**20**
C		**40**
D		**20**
Total		**100**

hydrogen 1 **H** 1.0079																		helium 2 **He** 4.0026
lithium 3 **Li** 6.941	beryllium 4 **Be** 9.0122												boron 5 **B** 10.811	carbon 6 **C** 12.011	nitrogen 7 **N** 14.007	oxygen 8 **O** 15.999	fluorine 9 **F** 18.998	neon 10 **Ne** 20.180
sodium 11 **Na** 22.990	magnesium 12 **Mg** 24.305												aluminium 13 **Al** 26.982	silicon 14 **Si** 28.086	phosphorus 15 **P** 30.974	sulfur 16 **S** 32.065	chlorine 17 **Cl** 35.453	argon 18 **Ar** 39.948
potassium 19 **K** 39.098	calcium 20 **Ca** 40.078		scandium 21 **Sc** 44.956	titanium 22 **Ti** 47.867	vanadium 23 **V** 50.942	chromium 24 **Cr** 51.996	manganese 25 **Mn** 54.938	iron 26 **Fe** 55.845	cobalt 27 **Co** 58.933	nickel 28 **Ni** 58.693	copper 29 **Cu** 63.546	zinc 30 **Zn** 65.39	gallium 31 **Ga** 69.723	germanium 32 **Ge** 72.61	arsenic 33 **As** 74.922	selenium 34 **Se** 78.96	bromine 35 **Br** 79.904	krypton 36 **Kr** 83.80
rubidium 37 **Rb** 85.468	strontium 38 **Sr** 87.62		yttrium 39 **Y** 88.906	zirconium 40 **Zr** 91.224	niobium 41 **Nb** 92.906	molybdenum 42 **Mo** 95.94	technetium 43 **Tc** [98]	ruthenium 44 **Ru** 101.07	rhodium 45 **Rh** 102.91	palladium 46 **Pd** 106.42	silver 47 **Ag** 107.87	cadmium 48 **Cd** 112.41	indium 49 **In** 114.82	tin 50 **Sn** 118.71	antimony 51 **Sb** 121.76	tellurium 52 **Te** 127.60	iodine 53 **I** 126.90	xenon 54 **Xe** 131.29
caesium 55 **Cs** 132.91	barium 56 **Ba** 137.33	57-70 *	lutetium 71 **Lu** 174.97	hafnium 72 **Hf** 178.49	tantalum 73 **Ta** 180.95	tungsten 74 **W** 183.84	rhenium 75 **Re** 186.21	osmium 76 **Os** 190.23	iridium 77 **Ir** 192.22	platinum 78 **Pt** 195.08	gold 79 **Au** 196.97	mercury 80 **Hg** 200.59	thallium 81 **Tl** 204.38	lead 82 **Pb** 207.2	bismuth 83 **Bi** 208.98	polonium 84 **Po** [209]	astatine 85 **At** [210]	radon 86 **Rn** [222]
francium 87 **Fr** [223]	radium 88 **Ra** [226]	89-102 * *	lawrencium 103 **Lr** [262]	rutherfordium 104 **Rf** [261]	dubnium 105 **Db** [262]	seaborgium 106 **Sg** [266]	bohrium 107 **Bh** [264]	hassium 108 **Hs** [269]	meitnerium 109 **Mt** [268]	ununnilium 110 **Uun** [271]	unununium 111 **Uuu** [272]	ununbium 112 **Uub** [277]		ununquadium 114 **Uuq** [289]				

*Lanthanide series	lanthanum 57 **La** 138.91	cerium 58 **Ce** 140.12	praseodymium 59 **Pr** 140.91	neodymium 60 **Nd** 144.24	promethium 61 **Pm** [145]	samarium 62 **Sm** 150.36	europium 63 **Eu** 151.96	gadolinium 64 **Gd** 157.25	terbium 65 **Tb** 158.93	dysprosium 66 **Dy** 162.50	holmium 67 **Ho** 164.93	erbium 68 **Er** 167.26	thulium 69 **Tm** 168.93	ytterbium 70 **Yb** 173.04
* *Actinide series	actinium 89 **Ac** [227]	thorium 90 **Th** 232.04	protactinium 91 **Pa** 231.04	uranium 92 **U** 238.03	neptunium 93 **Np** [237]	plutonium 94 **Pu** [244]	americium 95 **Am** [243]	curium 96 **Cm** [247]	berkelium 97 **Bk** [247]	californium 98 **Cf** [251]	einsteinium 99 **Es** [252]	fermium 100 **Fm** [257]	mendelevium 101 **Md** [258]	nobelium 102 **No** [259]


IT'S ANOTHER DAY OF USELESS WORK AND NO ACCOMPLISHMENT.
www.dilbert.com scottadams@aol.com
LUCKILY I HAVE A MEANINGFUL PERSONAL LIFE
10-31-06 ©2006 Scott Adams, Inc./Dist. by UFS, Inc.
RATBERT BROKE THE XBOX.
GAAA!!! I HAVE NOTHING!

Part A. (20 points, 2 points each)

PLEASE FILL IN THE BLANKS.

1. A type of secondary bond in which a temporary dipole induces another dipole in an adjacent atom is referred to as a ______ **van der Waals** ____________ bond.

2. The principle, known as the ___________ **Pauli exclusion** ______ principle, states that no two interacting electrons may have the same four values for their quantum numbers.

3. The primary bonds formed between atoms with large difference in electronegativity are referred to as ______ **ionic__bonds** __________________.

4. What symmetry elements does a water molecule have? Water possess two reflections planes and a C_2

5. The energy required to remove an electron from an isolated neutral atom is referred to as its _ **ionization potential** ___________________________________.

6. The ___ **hydrogen bond** ____________ is the strongest type of secondary bond.

7. A lattice together with its basis is referred to as the ________**crystal structure**_.

8. The ratio of the volume occupied by the atoms to the total available volume is defined to be the ____ **atomic packing factor** ___________________ for the crystal structure.

9. The term ___**liquid crystals**________________________ is given to fluids that show some degree of long-range order like molecular orientation.

10. The hard sphere, FCC (Face Centered Cubic) structure has the same packing density as what other close-packed structure? HCP

Part B. (20 points, 2 points each)

CIRCLE THE APPROPRIATE ANSWERS or WRITE THE ANSWERS AS REQUIRED

1. The coordination number of a(n) covalent / ionic bond is not simply determined by the radius ratio.

2. A lattice together with its basis is referred to as the unit cell / crystal structure .

3. How did we know that there are specific number of energy levels, say for H_2? With the use of spectral data obtained from atomic spectra

4. The lattice parameters of most metals are on the order of a few angstroms / nanometers .

5. Metals / ceramics / polymers have the highest density.

6. How many neutrons are there in an atom of the isotope ^{60}Co? [The atomic number is 27].

7. There is (are) **1 /** 4 atom(s) per lattice point in FCC nickel.

8. The Spatial distribution of the electrons in orbits can be influenced by external fields (true/false).

9. The secondary bonds between water molecules result from induced / permanent dipoles.

10. Nematic liquid crystals possess long-range orientational order/long-range positional order/possess no order.

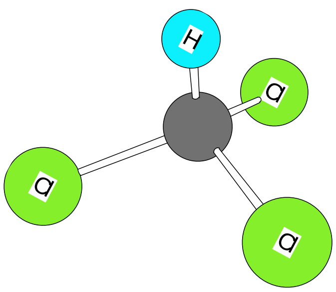
Part C. (40 points) ANSWER THE QUESTIONS

1. (10 Points) Symmetry is defined in terms of *elements* and *operations*: What are <u>all</u> the elements and operations?

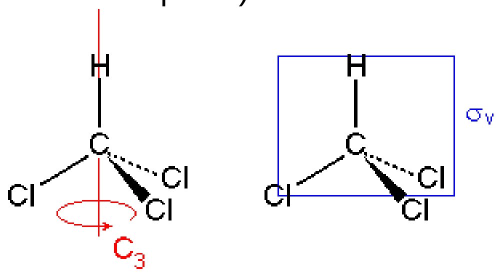
Element	**Operation**
Rotation axis, C_n	n-fold rotation
Improper rotation axis, S_n	n-fold improper rotation
Plane of symmetry, σ	Reflection
Center of symmetry, i	Inversion
	Identity, E

2. (10 Points) What ***symmetry elements*** and ***operations*** do these objects possess? (you may not get them all but please make an attempt)

One i, Center of inversion
One C_6 rotation axis perpendicular to the molecular plane
One C_3 rotation axis perpendicular to the molecular plane.
One C_2 rotation axis perpendicular to the molecular plane.
Three C_2' rotation axes in the molecular plane.
Three C_2'' rotation axes in the molecular plane.
One σ_h reflection plane corresponding to the molecular plane.
Three σ_v reflection planes containing the principal axis (C_6).
Three σ_d reflection planes containing the principal axis (C_6)
One S_6 improper axis coincident with the C_6 axis.
One S_3 improper axis coincident with the C_3 axis

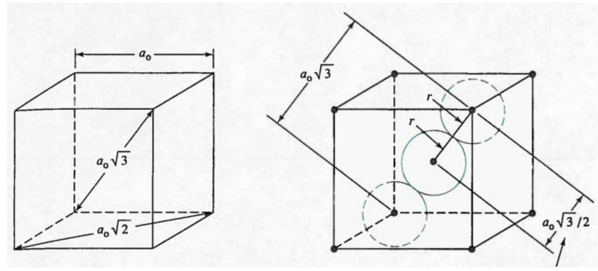


As shown in the figure below, there is a c_3 axis of rotation that passes through the C-H bond. It is also the principal axis of rotation. There are three σ_v mirror planes (each defined by the H-C-Cl bond plane).



Symmetry elements: E, C_3, σ_v, σ_v', σ_v''

3. (10 points) Calculate the length of a face diagonal of Cr, a BCC metal. The atomic radius of Cr = 1.25 Å.



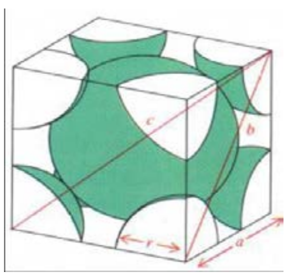
Answer:

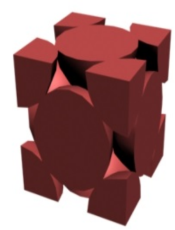
The length of the face diagonal is $\sqrt{2}\, a_o$. Atoms touch along the body diagonal, which has length $\sqrt{3}\, a_o = 4r$.

$\rightarrow \quad a_o = 4r / \sqrt{3}$

$\rightarrow \sqrt{2}\, a_o = 4r\sqrt{2} / \sqrt{3} = 4(1.25 \text{ Å})\sqrt{2} / \sqrt{3} = \underline{4.08 \text{ Å}}$

4. (10 points) Calculate the atomic packing factors for a BCC and an FCC structure.





See the pdf that is attached.

Part D. (20 points) ANSWER THE QUESTIONS

1. (5 Points) What are the relationships between the radius of the sphere and the dimension of the cube edge that are necessary to calculate the packing factor using the hard sphere approximation for the FCC and BCC structures? Sketch a figure to accompany your answer.

   For FCC see equation 3.3-2, page 68, and page 68 for the figure
   For BCC see equation 3.3-1, page 66, see page 67 for the figure

2. (5 Points)Show the packing factor for SC < BCC < FCC.

   For BCC see example problem 3.5-7
   For FCC see equation 3.5-3c

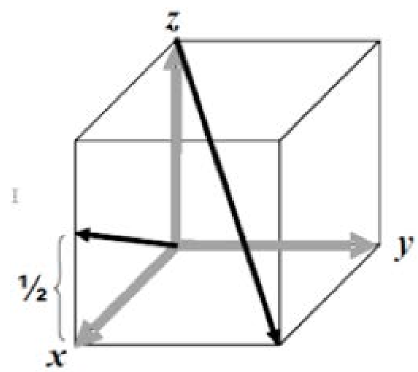
3. (**5 points, 2.5 points each**) Determine the Miller indices of the two directions shown in the figure below.

Solution:

For the first direction, use (0,0,0) as the point of origin:
x=1, y=0, z= ½. Clear the fractions to get [201]

For the second direction, use (0,0,1) as the point of origin:
x= 1, y=1, z=-1 or $[11\bar{1}]$

So the answer is **c)**



4. (5Points) Write Miller indices of the points, and directions, in the cubic cell shown below:

Point A:______________

Point B:______________

Direction C:___________

Direction D:___________