Ph.D. Qualifying Exam – May 21, 2013
Materials Science

There are five questions, one from each of the following sections: Thermodynamics, Advanced Materials, Solid State Physics, Smart Materials, and Diffraction.

Answer any four of the five questions.

Q1. Thermodynamics

Carnot Cycle

Given that: $dv(T, P) = v\,\alpha\, dT - v\,\beta\, dP$, $v = 1/\rho$, ρ = density

where $\alpha = (1/v)\ \partial v/\partial T\ _P$, coefficient of thermal expansion

$\beta = -(1/v)\ \partial v/\partial P\ _T$, isothermal compressibility

and noting: $c_p - c_v = T v\, \alpha^2/\beta$

(a) Determine: $ds\,(T, P)$, where $s(T, P)$ is the entropy.

(b) (i) Sketch the Carnot cycle in the P- v plane;
(ii) Determine analytically the slopes of the lines

Point Defects in Crystals

A monatomic crystal contains N_L lattice sites of which N are *occupied* and n are *vacant*.

(a) If the vacancies are randomly distributed, determine the entropy of the crystal

(b) Is your answer to part (a) the same as the entropy of mixing for an *ideal solution* composed of sites occupied by atoms and vacancies? Why?

(c) Considering the vacancies and atoms to actually be an *ideal mixture* of these two 'components', state whether the following 'total properties' are greater than, less than, or equal to zero:
(i) ΔH_{mix}
(ii) ΔS_{mix}
(iii) ΔG_{mix}

Q2. Advanced Materials

In a binary system of A and B atoms with the phases α and β in equilibrium at constant T, V, each change in F can be described as the sum of the changes in both phases. The physical quantities of the system are given below:

T: temperature
V: volume
F: Helmholtz free energy
n_i^α $(i = A, B)$: number of atoms of the component i ($i = A$, B) in α phase
n_i^β $(i = A, B)$: number of atoms of the component i ($i = A$, B) in β phase
μ_i^α $(i = A, B)$: the chemical potential of the component i ($i = A$, B) in α phase
μ_i^β $(i = A, B)$: the chemical potential of the component i ($i = A$, B) in β phase

We also have the following relationship:

$$dn_i = |dn_i^\alpha| = \left|-dn_i^\beta\right| \ (i = A, B)$$

Derive the equilibrium conditions of the system.

Q3. Solid State Materials Physics

Two-dimensional system. Suppose that we have free electrons in a two-dimensional quantum well with dimensions L x L.

(a) Write Schrödinger equation of a particle in the 2D well, to find expression of eigenfunction and available energy levels.

(b) What are the lowest and the second–lowest possible values for energy E, what is the degree of degeneracy for these energy states?

(c) Derive density of energy state for the 2D system. (Assume there are total N free electrons in the quantum well)

Q4. Smart Materials (100%)

(a) (14%) A semiconductor has an energy band gap of 1.1 eV. How many electron-hole pairs are generated when a photon of energy 2,600 eV is incident on the semiconductor?

(b) (14%) What is the wavelength of electromagnetic radiation with photon energy 1.1 eV?

The speed of propagation of the radiation is 3×10^8 m/s.

Planck's constant h = 0.6626×10^{-33} J.s.

1 eV = 1.9×10^{-19} J.

(c) (14%) Light travels from a medium with refractive index 1.57 to a medium with refractive index 1.35. Calculate the critical angle.

(d) (14%) A material of volume 1,700 cm^3 has a magnetization of 6.5×10^5 A/m. What is the magnetic moment of this material?

(e) (14%) What is the number of Bohr magnetons associated with an iron atom? The electronic configuration of iron is ...$3d^6$ $4s^2$.

(f) (14%) A piezoelectric material provides a strain of 1.89% under an applied electric field of 2,500 V/m. What is the piezoelectric coupling coefficient?

(g) (16%) Give the unit of each of the following quantities:

Contact electrical resistivity

Volume electrical resistivity (often simply called the electrical resistivity)

Mobility (in relation to electrical conduction)

Piezoelectric coupling coefficient

Q5. Diffraction (100%)

Below is the Periodic Table of the Elements.

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]

(a) (25%) Sketch the positive mass spectrum of Br-CH_3. Bromine has two isotopes with masses 79 and 81, such that they are about equal in abundance. For carbon, just consider the main isotope, which has mass number 12. For hydrogen, just consider the main isotope, which has mass number 1.

(b) (25%) Rutherford ion backscattering is conducted for a specimen in the form of a copper-silver-gold alloy thin film on a substrate. The projectile ion is $^4He^+$ (mass = 4 amu) at energy 2 MeV. The scattering angle is 180^0. (In practice, the scattering angle is less than 180^0, but it is taken to be 180^0 in this problem for the sake of ease of calculation.) When the scattering angle is 180^0, the kinematic recoil factor $k_M = [(M - m)/(M + m)]^2$, where m is the projectile ion mass and M is the target mass. Calculate the energy of the $^4He^+$ ions backscattered from the gold atoms at the very surface of the specimen. In addition, sketch the Rutherford ion backscattering spectrum (i.e., plot of ion yield vs. energy of the backscattered ion).

(c) (25%) Quantitative elemental analysis using x-ray spectroscopy is complicated by matrix effects (i.e., the presence of element B in the presence of element A that is being analyzed). Explain by giving the scientific origin.

(d) (25%) Give the Miller indices of the three lowest angle diffraction lines in order in increasing diffraction angle for each of the following powder materials.

Material with a simple cubic crystal structure
Material with a simple tetragonal crystal structure
Material with a simple hexagonal crystal structure
Material with a body-centered cubic crystal structure
Material with a face-centered cubic crystal structure