

**State University of New York
University at Buffalo
Department of Mechanical and Aerospace Engineering**

**Ph.D. Qualifying Examination in Materials Science
Jan. 25, 2008**

This test includes 8 problems on 5 pages. Please answer any **four** of these 8 problems in the blue book(s) provided. The attached Periodic Table of the Elements includes information on the atomic masses of the elements.

Problem 1 (100%)

Describe an effective experimental method for performing each of the following tasks.

- (a) (10%) Distinguishing between amorphous silicon and polycrystalline silicon.
- (b) (10%) Distinguishing between a metal and a semiconductor.
- (c) (10%) Distinguishing between the lead-rich and tin-rich phases in a tin-lead eutectic alloy.
- (d) (10%) Distinguishing between carbon monoxide gas and nitrogen gas.
- (e) (10%) Determining the thickness of a copper thin film on a silicon substrate.
- (f) (10%) Determining the energy band gap of a semiconductor.
- (g) (10%) Determining the phase of the copper-tin compound at the interface between tin and copper.
- (h) (10%) Determining the activation energy of the reaction between copper and tin.
- (i) (10%) Determining the frequency of a lattice vibrational mode of a material.
- (j) (10%) Determining the crystallographic texture of a metal sheet.

Problem 2 (100%)

Explain each of the following statements by giving the scientific origin.

- (a) (10%) A solid expands upon heating.

- (b) (10%) Diamond is an excellent thermal conductor.
- (c) (10%) The modulus of elasticity of a carbon fiber is higher along the axis of the fiber than in the transverse direction.
- (d) (10%) A semicrystalline polymer tends to be able to withstand higher temperatures than a conventional polymer.
- (e) (10%) An electrostrictive material strains in the presence of an electric field.
- (f) (10%) The yield stress of a magnetorheological fluid increases in the presence of a magnetic field.
- (g) (10%) A laser is superior to a light emitting diode as a light source for an optical fiber sensor.
- (h) (10%) An optical fiber sensor can be used to monitor the curing of epoxy.
- (i) (10%) A shape memory alloy can remember its shape.
- (j) (10%) The electrical resistivity of a metal increases with increasing temperature.

Problem 3 (100%)

The primitive translation vectors of a simple cubic lattice may be taken as:

$$\mathbf{a}=\mathbf{ax}; \mathbf{b}=\mathbf{bx}; \mathbf{c}=\mathbf{cx}, \text{ where } \mathbf{x}, \mathbf{y}, \text{ and } \mathbf{z} \text{ are unit vectors.}$$

What are the primitive translation vectors **A**, **B**, and **C** of its reciprocal lattice?

Problem 4 (100%)

Fig. 1 shows a simple method of estimating the theoretical shear strength of a perfect crystal. For small elastic strains, the stress σ is related to the displacement x by: $\sigma=Gx/d$, where d is the interplanar distance between atom in rows A and B, and G is the shear modulus (derived from the broken line in stress versus displacement at the initial slope). At first approximation, stress-displacement relation for large displacements may be written as:

$$\sigma=(Ga/2\pi d) \sin(2\pi x/d),$$

where 'a' is the interatomic spacing in the shear direction.

(a) (80%) What is the critical shear stress σ_c at which the lattice becomes unstable (that is when the atoms in row A are directly above B corresponding to zero stress)?

(b) (20%) What is the value of σ_c when $a \approx d$?

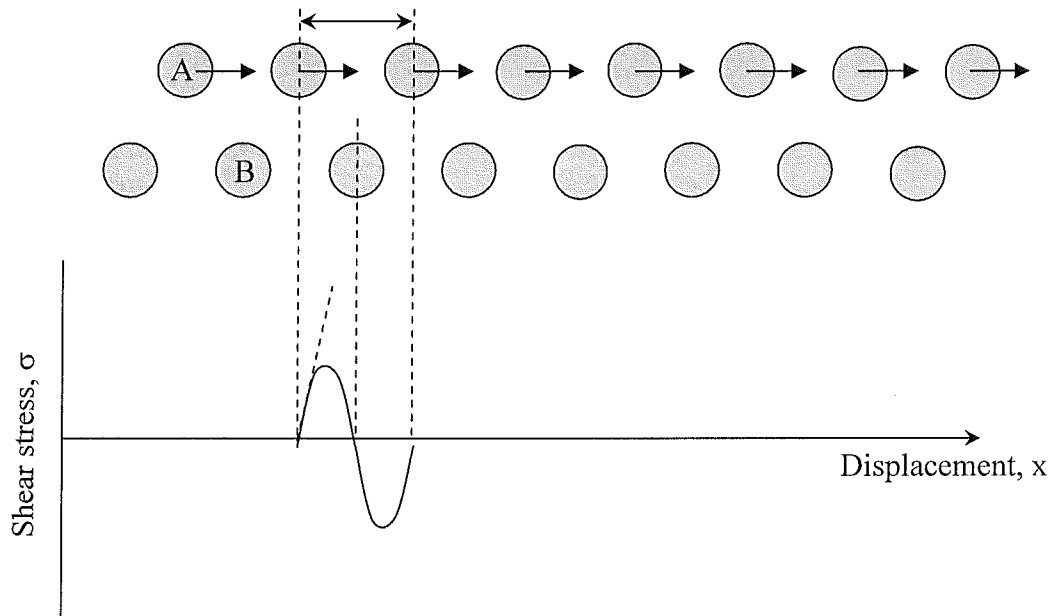


Fig. 1

Problem 5 (100%)

(a) (20%) Derive the Maxell relationships for Helmholtz energy, A ; Gibbs energy, G ; Enthalpy, H ; and Free energy, E .

(b) (60%) Show that $C_p - C_v = \alpha^2 VT / \beta$, where C_p and C_v are the respective heat capacities at constant pressure and volume, α is the coefficient of thermal expansion, β is compressibility, V is the volume of the system, and T is the temperature.

(c) (20%) What does this expression reduce to for the case of an ideal gas?

Problem 6 (100%)

Classical Thermodynamics – isotropic, non-ferromagnetic material.

The variation of the entropy, S , with temperature, T , and magnetic field, H , is given by:

$$dS(T, H) = \left(\frac{C_H}{T} \right) dT - (V\gamma_H) dH$$

where $C_H = (\delta Q_{\text{rev}} / dT)|_H$, heat capacity at constant magnetic field

and $\gamma_H = - (\partial B / \partial T)|_H$

Magnetic cooling is commonly used during the process of achieving sub-Kelvin temperatures. The procedure consists of the following steps:

Step 1. While being held *isothermal* at a low temperature (i.e., liquid helium, $T_0 = 4K$), the material is placed in a magnet whose *field strength* is *increased* to H .

Step 2. The material is *thermally insulated* while in the magnet and then the *field strength* is *reduced* to zero.

(a) In Step 1, write an expression for the heat transfer and determine whether the heat is flowing into or out of the material.

(b) Determine an expression for the temperature of the material after Step 2.

Problem 7 (100%)

Statistical Thermodynamics – crystal defects.

A Schottky defect is an intrinsic imperfection in a crystal lattice in which both a cation and anion site are vacant. To form this defect requires an energy ε . Consider the perfect

lattice as the 'ground state' with each site having an energy $\varepsilon_0 = 0$. Each Schottky defect then has an energy $\varepsilon_1 = \varepsilon$. There are N total sites in the crystal.

Nomenclature: (n_0, n_1) designate the number of sites having energies $(\varepsilon_0, \varepsilon_1)$, respectively;

U is the total crystal energy *above* the ground state;

T is the temperature (absolute)

Ω is the number of *microstates* corresponding to a given *macrostate*.

(a) Determine the entropy of the crystal, S , as a function of (U, ε, N) .

(b) Determine the energy of the crystal, U , as a function of (T, ε, N) .

(a) Determine the heat capacity of the crystal, C_v , as a function of (T, ε, N) .

Problem 8 (100%)

Classical Thermodynamics – binary solution.

The *partial molal heat of mixing* of species A associated with binary mixtures of A and B is given by:

$$\Delta \bar{H}_A = a_0 X_A X_B^2$$

where

$$X_i = \text{mole fraction of species } i$$

Determine the *heat of mixing*, $\Delta \bar{H}_{mix}$, in terms of X_A, X_B, a_0 .

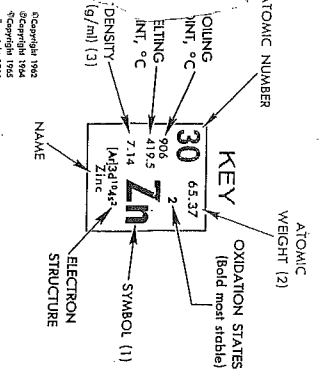
PERIODIC TABLE OF THE ELEMENTS

Table of Radioactive Isotopes

GROUP IA		GROUP IIA		GROUP IIIA		GROUP IVA		GROUP VA		GROUP VIA		GROUP VIIA		GROUP VIIIA		GROUP VIIIA	
1 H 1.00797 Hydrogen	2 He 4.0026 Helium	3 Li 6.939 Lithium	4 Be 9.0122 Beryllium	5 B 10.811 Boron	6 C 12.01115 Carbon	7 N 14.00642 Nitrogen	8 O 15.9994 Oxygen	9 F 18.9984 Fluorine	10 Ne 20.183 Neon	11 Na 22.989769 Sodium	12 Mg 24.312 Magnesium	13 Al 26.9815385 Aluminum	14 Si 28.0855 Silicon	15 P 30.973761998 Phosphorus	16 S 32.06 Sulfur	17 Cl 35.453 Chlorine	18 Ar 39.948 Argon
19 K 39.102 Potassium	20 Ca 40.08 Calcium	21 Sc 44.955912 Scandium	22 Ti 47.88 Titanium	23 V 50.9415 Vanadium	24 Cr 51.9961 Chromium	25 Mn 54.938 Manganese	26 Fe 55.847 Iron	27 Co 58.933 Cobalt	28 Ni 58.71 Nickel	29 Cu 63.546 Copper	30 Zn 65.37 Zinc	31 Ga 69.723 Gallium	32 Ge 72.64 Germanium	33 As 74.9216 Arsenic	34 Se 78.96 Selenium	35 Br 79.904 Bromine	36 Kr 83.80 Krypton
37 Rb 85.47 Rubidium	38 Sr 87.62 Strontium	39 Y 88.905848 Yttrium	40 Zr 91.224 Zirconium	41 Nb 92.90638 Niobium	42 Mo 95.94 Molybdenum	43 Tc 98 Technetium	44 Ru 101.07 Ruthenium	45 Rh 102.9055 Rhodium	46 Pd 106.42 Palladium	47 Ag 107.8682 Silver	48 Cd 112.404 Cadmium	49 In 114.818 Indium	50 Sn 118.610 Tin	51 Sb 121.757 Antimony	52 Te 127.60 Tellurium	53 I 126.90547 Iodine	54 Xe 131.30 Xenon
55 Cs 132.9054519 Cesium	56 Ba 137.327 Barium	57 La 138.90487 Lanthanum	58 Ce 140.12 Cerium	59 Pr 140.907647 Praseodymium	60 Nd 144.242 Neodymium	61 Pm 147 Promethium	62 Sm 150.35 Samarium	63 Eu 151.96 Europium	64 Gd 157.25 Gadolinium	65 Tb 158.925 Terbium	66 Dy 162.50 Dysprosium	67 Ho 164.93032 Holmium	68 Er 167.259 Erbium	69 Tm 168.934 Thulium	70 Yb 173.04 Ytterbium	71 Lu 174.967 Lutetium	
87 Fr (223) Francium	88 Ra (226) Radium	89 Ac (227) Actinium	90 Th 232.0377 Thorium	91 Pa (231) Protactinium	92 U 238.02891 Uranium	93 Np (237) Neptunium	94 Pu (242) Plutonium	95 Am (243) Americium	96 Cm (247) Curium	97 Bk (247) Berkelium	98 Cf (249) Californium	99 Es (254) Einsteinium	100 Fm (253) Fermium	101 Md (256) Mendelevium	102 No (254) Nobelium	103 Lw (257) Livermorium	

Neutral occurring radioactive isotopes are indicated by a blue mass number. Half lives are in parentheses where s, m, h, d and y stand for seconds, minutes, hours, days and years respectively. The symbols denoting the mode of decay and resulting radiation are defined as follows:

- α - alpha particle
- β^- - beta particle
- β^+ - positron
- K - K-electron capture
- L - L-electron capture
- SF - spontaneous fission
- γ - gamma ray
- IC - internal electron conversion



NOTES:
 (1) Black — solid.
 Red — gas.
 Blue — liquid.
 Purple — synthetically prepared.
 (2) Based upon carbon = 12. () indicates most stable or best known isotope.
 * Values for gaseous elements are for liquids at the boiling point.

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