State University of New York
University at Buffalo
Department of Mechanical and Aerospace Engineering
Ph.D. Qualifying Examination
Materials
May 14, 2009
Closed book

There are FIVE sections in this exam, A through E. Each section has two questions. Answer a total of FOUR questions. Each of the four answered question must be from a <u>different</u> section.

Section A: Diffraction, microscopy and spectroscopy techniques

<u>Problem 1</u> (100%)

A material exhibits the simple hexagonal crystal structure (i.e., a structure based on the hexagonal lattice with one atom in the basis), with lattice constant a = 3.87 Å and c = 4.28 Å.

(a) (10%) Give the Miller indices of the crystallographic plane with the highest planar density of atoms.

(b) (10%) What is the value of the largest interplanar spacing for this structure?

(c) (10%) Calculate the interplanar spacing for the (110) plane.

(d) (10%) What is the radius of an atom in this structure?

(e) (10%) What is the coordination number (the number of nearest atoms around an atom) for this structure?

(f) (10%) Give the Miller indices of the crystallographic plane that is perpendicular to the [010] direction.

(g) (10%) X-ray diffraction is conducted on a power specimen of this material, using a diffractometer and radiation of wavelength 1.542 Å. What is the angle of diffraction (2θ) for the lowest angle line in the diffraction pattern?

(h) (10%) X-ray diffraction is conducted on a single crystal specimen of this material, using a diffractometer and radiation of wavelength 1.542 Å. The specimen is oriented with the c-axis perpendicular to the plane of diffraction. Sketch the diffraction pattern and label each peak with its Miller indices. In the sketch, label the central reciprocal lattice point with the indices 000.

(i) (10%) Sketch the reciprocal lattice plane that is perpendicular to the c-axis. Label each reciprocal lattice point with its Miller indices.

(j) (10%) Calculate the volume of the primitive unit cell in reciprocal space.

<u>Problem 2</u> (100%)

Provide a very brief answer to each of the following 20 questions.

(i) (5%) In relation to the information that can be obtained, what is the main advantage of scanning electron microscopy compared to transmission electron microscopy?

(ii) (5%) In relation to the information that can be obtained, what is the main advantage of transmission electron microscopy compared to scanning electron microscopy?

(iii)(5%) In relation to the information that can be obtained, what is the main advantage of fractography compared to metallography?

(iv)(5%) In relation to the information that can be obtained, what is the main advantage of dark-field transmission electron microscopy compared to bright-field transmission electron microscopy?

(v) (5%) In relation to the information that can be obtained by scanning electron microscopy, what is the main advantage of imaging using secondary electrons compared to imaging using backscattered electrons?

(vi)(5%) In relation to the information that can be obtained by scanning electron microscopy, what is the main advantage of imaging using backscattered electrons compared to imaging using secondary electrons?

(vii) (5%) In relation to the information that can be obtained, what is the main advantage of scanning transmission electron microscopy compared to transmission electron microscopy?

(viii) (5%) In relation to the information that can be obtained, what is the main advantage of scanning Auger microscopy compared to scanning electron microscopy?

(ix)(5%) In relation to the information that can be obtained, what is the main advantage of atomic force microscopy compared to scanning tunneling microscopy?

(x) (5%) In relation to the information that can be obtained, what is the main advantage of electron microprobe compared to x-ray fluorescence?

(xi)(5%) In relation to the information that can be obtained, what is the main advantage of x-ray photoelectron spectroscopy compared to ultraviolet photoelectron spectroscopy?

(xii) (5%) In relation to the information that can be obtained, what is the main advantage of ultraviolet photoelectron spectroscopy compared to x-ray photoelectron spectroscopy?

(xiii) (5%) In relation to the information that can be obtained, what is the main advantage of infrared spectroscopy compared to ultraviolet spectroscopy?

(xiv) (5%) In relation to the information that can be obtained, what is the main advantage of mass spectrometry compared to atomic absorption spectroscopy?

(xv) (5%) In relation to the information that can be obtained from mass spectrometry, what is the main advantage of a high-magnetic-field mass spectrometer compared to a low-magnetic-field mass spectrometer?

(xvi) (5%) In relation to the information that can be obtained, what is the main advantage of high energy (Rutherford) ion backscattering compared with low energy ion backscattering.

(xvii) (5%) In relation to the information that can be obtained from light scattering, what is the main advantage of Raman scattering compared to Rayleigh scattering?

(xviii) (5%) In relation to the information that can be obtained, what is the main advantage of electron diffraction compared to x-ray diffraction?

(xix) (5%) In relation to the information that can be obtained from x-ray diffraction, what is the main advantage of powder diffraction compared to single crystal diffraction?

(xx) (5%) In relation to the information that can be obtained from x-ray diffraction, what is the main advantage of the Laue method compared to the diffractometer method?

Section B: Smart materials

<u>Problem 1</u> (100%)
A dielectric material is in the form of a disc of thickness 30 μm and diameter 750 μm. In the direction perpendicular to the plane of the disc, the material exhibits electrical resistivity 3500 Ω.cm (1 kHz) , relative dielectric constant 45 (1 kHz), piezoelectric coupling coefficient d 120 x 10^{-12} m/V (1 kHz), and elastic modulus 535 GPa.
Permittivity of free space ε_o = 8.85 x 10^{-12} C/V.m

(i) (10%) Calculate the capacitance in the absence of an applied stress.

(ii) (10%) An electric field of 7.4 x 10^6 V/m is applied in the direction perpendicular to the plane of the disc. Calculate the polarization in the absence of an applied stress.
Hint: $P = (\kappa - 1)\ \varepsilon_o E$

(iii)(10%) Calculate the change in polarization due to an applied stress of 4.0 x 10^8 Pa in the direction perpendicular to the plane of the disc. Hint: $\Delta P = d\ U$, where U is the stress and d is the piezoelectric coupling coefficient.

(iv)(10%) A stress wave rather than a step change in stress is typically used to observe the direct piezoelectric effect. Why?

(v) (10%) What is the piezoelectric voltage coefficient g in the direction perpendicular to the plane of the disc? Hint: $g = 1/(Md)$, where M is the modulus.

(vi)(10%) Calculate the resistance in the direction perpendicular to the plane of the disc.

(vii) (10%) For a given open-circuit voltage output of the piezoelectric effect, the maximum power that can be generated is higher when the resistance is lower. Why?

(viii) (10%) Calculate tan δ (1 kHz) by considering an equivalent circuit with the resistor and capacitor parts of the dielectric material being in series. Hint: tan $\delta = \omega RC$

(ix)(10%) In general, tan δ depends on the frequency. Describe this frequency dependence.

(x) (10%) What is the physical meaning of the imaginary part of the relative dielectric constant?

Problem 2 (100%)

An electromagnetic interference (EMI) shield exhibits shielding effectiveness 26 dB, linear absorption coefficient 18 cm^{-1}, relative magnetic permeability 76, electrical resistivity 1.2×10^{-3} Ω.cm, and thickness 1.9 cm. The power of the incident beam is 46 mW.

Permeability of free space $\mu_o = 4\pi \times 10^{-7}$ H/m

(i) (12%) What is the power after transmission through the shield?

(ii) (12%) What is the absorption loss (in dB) due to the entire thickness of the shield?
Hint: Absorption loss (dB) = (10 / 2.3) αx

(iii)(12%) The reflection loss is 2.2 dB. What is the power of the reflected beam?

(iv)(14%) Calculate the skin depth at 1.0 GHz. Hint: $\delta = 1/\sqrt{(\pi \nu \mu \sigma)}$.

(v) (10%) What are the two main mechanisms of EMI shielding in general?

(vi)(10%) Why are nickel nanofibers of diameter 0.4 μm more effective than nickel fibers of diameter 2 μm for EMI shielding?

(vii) (10%) Why is cement a more effective matrix than polymer for providing composite materials for EMI shielding? The polymer is a conventional one – not an inherently conductive polymer.

(viii) (10%) What are the main criteria that govern the effectiveness of a material for low-observable aircraft?

(ix)(10%) Why is it that a metal detector can detect metals but not polymers or ceramics?

Section C: Advanced Materials Science

Problem 1 (100%) Assume that there exist two parallel dislocations in a solid material. The character of one is pure edge and the other is pure screw. Consider the interaction between the dislocations and use the corresponding elastic fields in the material to explain whether one dislocation exerts a force on the other.

Problem 2 (100%)

(a) There are three slip systems on a fcc octahedral plane. Assume 2 MPa tensile stress is applied along the [100] direction of a gold crystal, whose critical resolved shear stress is 0.91 MPa. Quantitatively show whether measurable slip will occur or not on any of the three slip systems in the (111) plane as a result of this applied stress. (50%)

(b) The total line length of the dislocations in a 4 cm by 4 cm TEM photograph, of a metal foil, taken at a magnification of 25,000 times is 400 cm. The foil imaged by the picture had a thickness of 300 nm. Determine the dislocation density in the foil (in terms of length of dislocation per unit volume of the foil). (50%)

Section D: Modern Theory of Materials

__**Problem 1 (100%)**__ We consider a crystalline nano wire. Assume that the wire can be approximately regarded as a one-dimensional atomic chain with a lattice spacing β between two adjacent atoms. The potential of atoms is represented by $V(x) = \beta V_0 \delta(x)$; here $\delta(x)$ is the Dirac-delta function. Please derive the single-atom ground-state wavefunction of the wire.

__**Problem 2 (100%)**__ For a diatomic linear chain, the phonon dispersion relation $\omega(q)$ has two branches shown below

$$\omega^2 = f\left(\frac{1}{m} + \frac{1}{M}\right) \pm f\left[\left(\frac{1}{m} + \frac{1}{M}\right)^2 - \frac{4}{mM} sin^2 \frac{qa}{2}\right]^{1/2}.$$

There are two atoms in the unit cell with masses M and m, and the force constant of the nearest-neighbor interaction is given by f.

(a) Calculate the sound velocity.
(b) Consider two cases: (1) $M = 10m$; (2) $M = m$. Discuss the dispersion relation $\omega(q)$ under these conditions.

Section E: Thermodynamics of Engineering Materials

Problem 1 (100%)

Consider a thermo-elastic solid subjected to uniaxial normal stress, σ_{xx} . The isothermal compressibility, β, is given by:

$$\beta \equiv (1/V)(\partial V / \partial \sigma_{xx})_T = (1-2\nu)/E$$

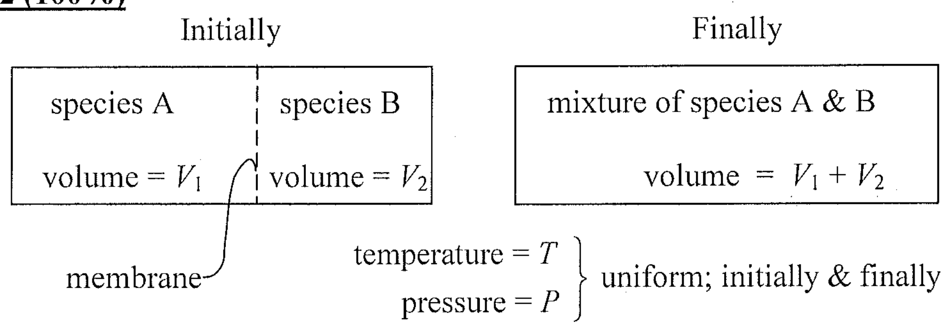
where ν is Poisson's ratio (constant) and E is the elastic modulus. The elastic modulus depends on temperature according to:

$$E(T) = E_0\,(1-t^3)$$

where $t \equiv (T-T_0)/(T_m - T_0)$; T_m is the melting temperature; E_0, T_0 are constants.

Determine $(\partial \alpha / \partial \sigma_{xx})_T$ where α is the coefficient of thermal expansion.

Problem 2 (100%)



(50%) (a) Both species are IDEAL GASES.

(20%) (i) What is the *heat of mixing*, ΔH_{mix} ?

(30%) (ii) From statistical thermodynamics, the entropy of *independent* particles may be written as:

$$S = U/T + kN \ln Z$$

where: U = internal energy, N = # particles, k = Boltzmann's const.
and Z = molecular partition function, which may be written as $= V\,f(T$, molecular constants)

Determine the *entropy of mixing*, ΔS_{mix} .

(50%) (b) Both species are LIQUIDS.

(25%) (i) If the two liquids form an *ideal mixture*, what are ΔH_{mix} and ΔS_{mix} ?

(25%) (ii) If the two liquids form a *regular mixture*, how do ΔH_{mix} and ΔS_{mix} compare to the same quantities for an *ideal mixture* ?
