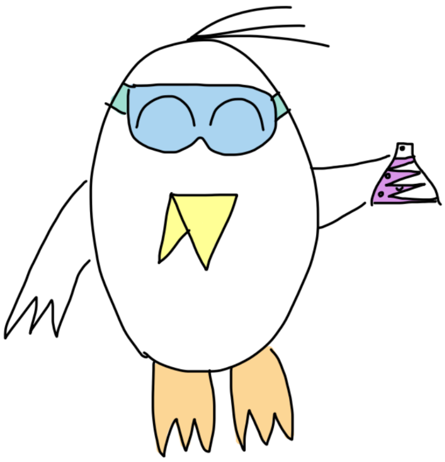
'Iolani Science Olympiad Invitational 2024

Division C

MATERIALS SCIENCE TEST KEY



Team Name ____

Team Number __________

Honolulu
2024

1 Calculations

1. (1 point) Identify the Bravais lattice corresponding to the dihedral point group with a 3-fold rotation axis, 3 twofold axes perpendicular to that axis, and 3 vertical mirror planes which pass between twofold axes.

Rhombohedral (also accept hexagonal). The Schoenflies notation for the rhombohedral lattice is D_{3D}.

2. (1 point) How many Bravais lattices are there in 4 dimensions?

64

3. (2 points) A metal has a face-centered cubic structure with a lattice parameter of 4.00 Angstroms. The atomic mass is 58.7 g/mol. Calculate the density for this metal. Give your answer in SI units. The mass of each atom m can be found from the atomic mass M by diving by Avogadro's number. There are four atoms in a unit cell, so the mass of the unit cell is $4\frac{M}{N_A}$. The volume of the unit cell is a^3 where a is the lattice parameter. Therefore the density is $\rho = \frac{4M}{N_A a^3}$. Plugging these values in, we get $\boxed{\rho = 6090 kg/m^3}$.

4. (4 points) Consider a monochromatic x-ray beam with a wavelength $\lambda =$ 0.154 nm (characteristic of Cu K-alpha radiation) incident on a crystalline material known to have a cubic structure with a lattice constant 0.4 nm. The beam is directed at a set of crystallographic planes indexed by their Miller indices (h, k, l).

(a) Determine the first-order Bragg angle for the $(1, 1, 1)$ planes. Provide your answer in degrees. We use the Bragg formula $n\lambda = 2d \sin\theta$. We find that $d = \frac{1}{\sqrt{1^2+1^2+1^2}} = \frac{\sqrt{3}}{3}$. Since $n = 1$, plugging values in gives us $\boxed{\theta = 19.47 \text{ degrees}}$.

(b) For the same crystal, the intensity of the reflected x-ray is measured to be maximum at $\theta = 25.6°$. Calculate the Miller indices of the planes responsible for this diffraction, considering only diffracted x-rays of the first order. We use the Bragg formula once more, except this time we wish to solve for d, which we find to be about $\frac{\sqrt{5}}{5}$. The only permissible values for (h, k, l) are $\boxed{(\pm 2, \pm 1, 0)}$, in any order.

5. (2 points) Niobium has the body-centered cubic crystal structure. Given that the density of Nb is 8,570 kg/m^3, and the atomic weight is 92.91 g/mole, what is the atomic radius (in pm) and the lattice parameter of Nb?

The density is equal to the mass of atoms in the unit cell divided by the volume of the unit cell. In a BCC structure, there are two atoms per unit cell, so the mass of atoms in the unit cell in terms of atomic weight M, is $2\frac{M}{N_A}$. The volume of the unit cell is a^3; rearranging for a, we have $a = \sqrt[3]{\frac{2M}{N_A \rho}}$, which we calculate to be $\boxed{a = 330.2 \text{ pm}}$. For a BCC structure, the relationship between the lattice parameter and atomic radius is $a = \frac{4r}{\sqrt{3}}$, which we can solve to discover that $\boxed{r = 143.0 \text{ pm}}$.

6. (2 points) Titanium diboride, important ceramic material, has a composition of two B atoms for every Ti atom. What weights of Ti and B must be mixed

together to make a 100g ingot of TiB_2? The atomic weights are Ti=47.88 g/mol, B=10.81 g/mol, and the densities are Ti=4.51 g/cc and B=2.34 g/cc.

The chemical formula TiB_2 indicates that the molar mass of TiB_2 is equal to the atomic mass of Ti plus twice the atomic mass of B, which we find to be 69.50 g/mol. The mass fraction of titanium is the atomic mass of titanium divided by the molar mass of the compound, and the mass fraction of boron is twice the atomic mass of boron divided by the molar mass of the compound. Multiplying this by the mass of the sample gives us the weights: $\boxed{\text{68.6 g titanium, 31.4 g Boron}}$.

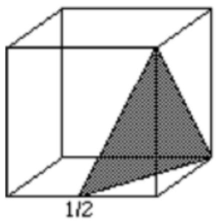
7. (1 point) In a typical X-ray crystallography experiment, X-rays of wavelength 0.71 Angstroms are generated by bombarding molybdenum metal with an energetic beam of electrons. Why are these X-rays more effectively diffracted by crystals than is visible light?

The x-rays are about the size as the atomic spacing

8. (1 point) What is the closest-packed plane in BCC? Give your answer in Miller indices.

(1 1 0)

9. (2 points) Draw a plane with Miller indices (-2,-1,1).



10. (3 points) You are given a material and told that it is elastically isotropic and exhibits a yield strength of 950 MPa. The material experiences a stress state of

$$\sigma_{ij} = \begin{bmatrix} 0 & 0 & 300 \\ 0 & -400 & 0 \\ 300 & 0 & -800 \end{bmatrix} \text{ MPa}$$

According to the von Mises and Tresca criteria respectively, does the material yield? Justify your answer.

The principal stresses are the eigenvalues of the given stress tensor; computing yields σ_1=-900 MPa, σ_2=-400 MPa, and σ_3= 100MPa. The von Mises criterion is $\sigma_{vM} = \sqrt{\frac{1}{2}\left[(\sigma_1-\sigma_2)^2+(\sigma_2-\sigma_3)^2+(\sigma_3-\sigma_1)^2\right]} = \boxed{866 \text{ MPa}}$, which is below the yield strength. The Tresca criterion is $\max(\sigma_i - \sigma_j) = \sigma_3 - \sigma_1 = \boxed{1000 \text{ MPa}}$, which is above the yield strength. Therefore, according to the von Mises criterion, the material will not yield, but according to the Tresca criterion, the material would fail.

11. (1 point) A borosilicate glass plate has a thermal expansion coefficient of $3.3 \times 10^{-6}\text{K}^{-1}$, Young's modulus of 64 GPa, and fracture strength of 50 MPa. calculate the maximum temperature difference the glass can withstand without breaking.

Thermal stress is given by $\sigma = E\alpha\Delta T$ with Young's modulus E, thermal expansion coefficient α, and temperature difference ΔT. The maximum ΔT, then, is the one for which the stress is equal to the fracture strength. Therefore $\Delta T = \frac{\sigma_{\text{fracture}}}{E\alpha} = \boxed{236.7 \text{ K}}$.

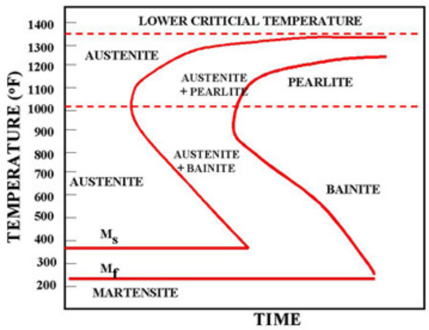
12. (2 points) Calculate the dielectric constant of a glass material with a polarizability of $\alpha = 1.0 \times 10^{-40}$ F$\cdot$m^2 and a number density of dipoles $N = 2.5 \times 10^{28}$ m^{-3}.

The Clausius Mossotti relation relates the dielectric constant ε_r of a material to its polarizability α and the number density of dipoles N: $\frac{\varepsilon_r - 1}{\varepsilon_r + 2} = \frac{N\alpha}{3\varepsilon_0}$. Rearranging and solving, the dielectric constant is $\varepsilon_r = 1.31$

13. (1 point) What is the molar heat-capacity of a solid crystalline substance as predicted by the Dulong-Petit law?

The Dulong-Petit law predicts that for a solid crystalline material, the molar heat capacity is $\boxed{\text{3R per mole of substance}}$, where R is the ideal gas constant.

14. (2 points) Given the TTT diagram below, percentage the fraction of pearlite transformed in a eutectoid steel isothermally held at 700 C for 5 seconds. Assume an Avrami exponent $n = 2$ and a rate constant $k = 0.05\text{s}^{-1}$. We use the



Avrami equation $f = 1 - \exp[(] - kt^n)$ where f is the fraction transformed, k is the rate constant, t is the time, and n is the Avrami exponent. Plugging in yields $\boxed{71.35\%}$.

15. (2 points) A ceramic material is studied as a potential high-temperature superconductor. Within the material, electrons are modeled as confined to a 2D potential well (representing the crystal plane) with an effective mass $m = 0.2m_e$, where m_e is the mass of the free electron. The dimensions of the potential well are $L_x = 0.5$ nm and $L_y = 0.3$ nm. Determine the wavelength of a photon required to excite the electron from the ground state to the first excited state, in nanometers.

The energy levels for a 2D potential well are given by $E_{n_x,n_y} = \frac{\hbar^2}{2m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2}\right)$. The ground state corresponds to $n_x = 1, n_y = 1$, and the first excited state corresponds to the next highest energy level, which would be $n_x = 2, n_y = 1$. The energy difference is then $\Delta E = \frac{\hbar^2}{2m}\left(\frac{3}{L_x^2}\right)$. Since the energy of a photon is related to its wavelength by $\Delta E = \frac{hc}{\lambda}$ we can rearrange to find that $\lambda = \boxed{542.72 \text{ nm}}$.

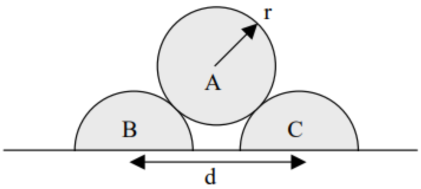
16. (2 points) Consider a single crystal of BCC iron oriented such that a tensile stress is applied along a [010] direction. If slip occurs on a (110) plane and in a $[\bar{1}11]$ direction, and the critical resolved shear stress is 30 MPa, calculate the magnitude of applied tensile stress necessary to initiate yielding. The single crystal plastically deforms or yields when the shear stress is the critical resolved

shear stress, and we determine the yield strength by $\sigma_y = \frac{\tau_{crss}}{(\cos\phi\cos\lambda)_{max}}$ where ϕ is the angle between the normal to the slip plane and the applied stress direction, and λ is the angle between the slip and stress directions. In general, for cubic unit cells, the angle between the directions $[u_1v_1w_1]$ and $[u_2, v_2, w_2]$ is given by $\cos^{-1}\left[\frac{u_1u_2+v_1v_2+w_1w_2}{\sqrt{(u_1^2+v_1^2+w_1^2)(u_2^2+v_2^2+w_2^2)}}\right]$. Using $[u_1v_1w_1] = [110][u_2v_2w_2] = [010]$, we have $\phi = 45°$. For λ, we take $[u_1v_1w_1] = [\bar{1}11]$ and $[u_2v_2w_2] = [010]$, which yields $\lambda = 54.7°$. Using our equation for σ_y we get $\boxed{73.4 \text{ MPa}}$.

17. (2 points) Silicon and Gallium Arsenide crystals can be described by an FCC lattice with two atoms per unit cell. The primitive vectors of the FCC lattice expressed in the Cartesian basis are given by $\vec{a}_1 = \frac{a}{2}(0,1,1)$, $\vec{a}_2 = \frac{a}{2}(1,0,1)$, $\vec{a}_3 = \frac{a}{2}(0,1,1)$ with a the lattice parameter. The basis vectors that describe the positions of atoms inside the unit cell are given by $\vec{\tau}_1 = \frac{a}{4}(1,1,1)$ and $\vec{\tau}_2 = -\frac{a}{4}(1,1,1)$. Find the reciprocal space primitive vectors.

In general, the primitive basis vectors in reciprocal space are given by $\vec{b_1} = 2\pi\frac{\vec{a_2}\times\vec{a_3}}{\vec{a_1}\cdot(\vec{a_2}\times\vec{a_3})}$, $\vec{b_2} = 2\pi\frac{\vec{a_3}\times\vec{a_1}}{\vec{a_1}\cdot(\vec{a_2}\times\vec{a_3})}$, $\vec{b_3} = 2\pi\frac{\vec{a_1}\times\vec{a_2}}{\vec{a_1}\cdot(\vec{a_2}\times\vec{a_3})}$. Calculating those cross products gives us $\boxed{\vec{b}_1 = \frac{2\pi}{a}(-1,1,1), \vec{b}_2 = \frac{2\pi}{a}(1,-1,1), \vec{b}_1 = \frac{2\pi}{a}(1,1,-1)}$

18. (3 points) A circular cylinder A rests on top of two half-circular cylinders B and C, all having the same radius r. The weight of A is W, and that of B and C is W/2 each. Assume that the coefficient of friction between the flat surfaces of the half-cylinders and the horizontal table top is μ_s. Determine the maximum distance d between the centers of the half cylinders to maintain equilibrium. The answer is $\boxed{d = 4\pi\sin\left(\tan^{-1}\mu_s\right)}$; the solution to this classic problem can be found here.



19. (3 points) You're building a small-scale wooden electrical vehicle, and you're in a hurry to get it done quickly before impound (you woke up at 4AM with nothing but a motor and an Arduino). Part of the model needs to be a structural member that has a length L and a square cross-section with side length L/10, and this structural member will be loaded in tension. At the last minute, you realize that you don't have any pieces of wood that are long enough; your longest pieces have a length of 0.8L. You do, however, have a bottle of glue that you can use to glue two pieces together to get the total length that you need. Your glue can withstand 1MPa of shear stress and 3MPa of normal stress. You also have a saw that you can use to cut the ends of the pieces of wood at any angle that you like prior to gluing. At what angle θ should you cut the wood faces if you want the resulting beam to be able to withstand the largest possible tensile load? (You can only cut a straight cut). The stress normal to the glue joint is $\sigma_n = \frac{2T\cos\theta}{A} \leq 3$ MPa, where T is the tensile load and A is the cross sectional area; the shear to the glue joint is $\sigma_s = \frac{2T\sin\theta}{A} \leq 1$ MPa. To maximize T

without exceeding the glue's stress limits we set the two stress conditions equal, so that 3 MPa $= \frac{1 \text{ MPa}}{\tan\theta}$. Solving, we get $\boxed{\theta \approx 18.43 \text{ degrees}}$.

20. (4 points) Consider a cylindrical tank of radius 1 m, length 2 m, and wall thickness 3 cm made of an isotropic linear elastic material with modulus 100 GPa and Poisson's ratio 0.3. The tank fits without stress between a rigid wall and a rigid plate when there is no pressure in the tank. A spring with spring constant 1 giganewton per meter fits exactly between the rigid plate and a second rigid wall. The plate can only move in the horizontal direction. The internal pressure in the tank is brought to a value 500 MPa. Obtain the resulting displacement of the plate and the change in wall thickness. The force also exerted by the tank due to pressure is $F = p\pi R^2$, which, using Hooke's law $F = -k\Delta x$, we can use to determine that the spring displacement due to the pressure is $\boxed{1.57 \text{ m}}$. The expression for the change in wall thickness is more involved; for this thin-walled cylindrical vessel the stresses are the hoop stress $\sigma_h = \frac{pR}{t}$ and axial stress $\sigma_a = \frac{pR}{2t}$ where p is pressure, R is radius, and t is thickness. Using the stress-strain relationships for isotropic materials, the hoop strain is $\epsilon_h = \frac{\sigma_h}{E} - \nu\frac{\sigma_a}{E}$ and the axial strain is $\epsilon_a = \frac{\sigma_a}{E} - \nu\frac{\sigma_h}{E}$. The radial strain is $\epsilon_r = -\nu(\epsilon_h + \epsilon_a)$, and the change in thickness is $\Delta t = \epsilon_r t = \boxed{-1.575 \text{ mm}}$.

2 Multiple choice

Each problem is worth 1 point. 1. During the sol-gel process for fabricating ceramic or glass materials, which of the following factors most significantly impacts the final pore structure of the material?

(a) Type of precursor used (e.g., alkoxides vs. nitrates)

(b) The water-to-alkoxide molar ratio during hydrolysis

(c) The curing temperature used before sintering

(d) The duration of the aging process of the gel

2. In tape casting, which of the following additives is primarily responsible for controlling the viscosity of the ceramic slurry?

(a) Binder

(b) Plasticizer

(c) Dispersant

(d) Solvent

3. Which of the following techniques is NOT typically used to reduce the sintering temperature of ceramic materials?

(a) Addition of a fluxing agent

(b) Spark plasma sintering

(c) Increasing the green density

(d) Using a higher cooling rate after firing

4. In the Czochralski process for producing single-crystal glass, what is the primary role of the rotation of the seed crystal?

(a) Prevent thermal gradients from cracking the crystal

(b) Promote uniform crystal growth by reducing solute boundary layers

(c) Control the incorporation of dopants into the crystal

(d) Align the crystal structure with the pulling direction

5. During the hot isostatic pressing (HIP) of ceramics, which factor is most critical for eliminating closed porosity without causing abnormal grain growth?

(a) The applied gas pressure

(b) The sintering atmosphere composition

(c) The heating rate during the process

(d) The temperature-holding time at peak pressure

6. In slip casting, which of the following defects is most likely caused by improper deflocculation of the slurry?

(a) Warping during drying

(b) Weak mechanical strength after sintering

(c) Non-uniform thickness of the green body

(d) Excessive cracking during the drying stage

7. Which phenomenon is most responsible for the increased mechanical strength observed in tempered glass?

(a) Decrease in residual thermal stresses due to quenching

(b) Compressive stresses introduced at the surface during cooling

(c) A transition from amorphous to partially crystalline structure

(d) Increased density of covalent bonding in the silica network

8. In the additive manufacturing (3D printing) of ceramics, which of the following methods typically achieves the highest density in the final product after post-processing?

(a) Binder jetting

(b) Vat photopolymerization

(c) Material extrusion

(d) Laser sintering

8. Which of the following steps in the fabrication of zirconia-toughened ceramics most directly contributes to the transformation toughening mechanism?

(a) Sintering at temperatures above the monoclinic phase stability range

(b) Rapid cooling to retain the tetragonal phase in the final product

(c) Inclusion of yttria as a stabilizer during powder preparation

(d) Homogenizing the initial powder blend to eliminate impurities

10. In the float glass process, what is the primary purpose of using molten tin in the fabrication of flat glass sheets?

(a) To enhance the thermal conductivity of the glass during annealing

(b) To achieve a perfectly flat surface without grinding or polishing

(c) To reduce the melting temperature of the silica precursor

(d) To provide a nucleation site for glass crystallization