Materials Science C

November 15-23, 2025

Instructions:

- ➔ You will have **50 minutes** to complete your exam. At the end of this time period, you must stop working. Partial credit will be awarded, so attempt as many questions as you can, and show your work!
- ➔ **Reference Materials:** Please follow national Science Olympiad rules for reference materials. Do not consult the internet, artificial intelligence, or any outside sources.
- ➔ **Calculator:** You may use a Class III graphing calculator (see Science Olympiad rules for calculator classes)
- ➔ This test is graded out of **120 points.** The highest score wins.
- ➔ Have fun!

School/Team Name: _____

Team Number: ____

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1 Multiple-Choice Questions (26 points)

1. (1 point) The theoretical maximum packing efficiency of the hexagonal close-packed structure is:
   A. 67.0%
   B. 74.0%
   C. 52.4%
   D. 80.0%

2. (1 point) Which pair of elements would exhibit the greatest degree of covalent character according to Pauling's scale of electronegativity?
   A. Na-Cl
   B. Si-O
   C. Mg-F
   D. Al-N

3. (1 point) The Born exponent n is the Born-Mayer potential is most closely related to:
   A. The compressibility of the crystal
   B. The ionic radii ratio
   C. The polarizability of the anion
   D. The bond dissociation energy at zero separation

4. (1 point) A polycrystalline metal contains a tilt boundary formed by an array of edge dislocations. The grain boundary energy per unit area depends on the misorientation angle θ. If the grain boundary energy is 200 mJ/m^2 at $\theta = 5°$, which of the following best described the expected energy at $\theta = 10°$?
   A. Exactly 400 mJ/m^2
   B. Less than 400 mJ/m^2
   C. Greater than 400 mJ/m^2
   D. Exactly 200 mJ/m^2

5. (1 point) Which imperfection introduces tensile stress fields in the surrounding lattice?
   A. Interstital atom
   B. Vacancy
   C. Edge dislocation extra half-plane
   D. Screw dislocation

6. (1 point) The burgers vector $\mathbf{b}$ of a perfect dislocation in a BCC metal is:
   A. $a\langle 100\rangle$
   B. $\frac{a}{2}\langle 111\rangle$
   C. $a\langle 110\rangle$
   D. $\frac{a}{2}\langle 110\rangle$

7. (1 point) Diamond has $k \sim 2000$ W m^{-1} K^{-1}, $\rho = 3500$ kg/m^3, $c_p = 500$ J kg^{-1} K^{-1}. Its thermal diffusivity is roughly:
   A. 10^{-8} m^2/s
   B. 10^{-5} m^2/s
   C. 10^{-4} m^2/s

D. 10^{-3} m^2/s

8. (1 point) Zirconium tungstate (ZrW_2O_8) exhibits isotropic negative thermal expansion over a broad temperature range. This counter-intuitive behavior is primarily due to:
   A. Rigid-unit transverse vibrations of WO_4 and ZrO_6 polyhedra
   B. Electronic delocalization upon heating
   C. Cation–anion size-mismatch strain relief
   D. Magnetostrictive domain reorientation

9. (1 point) In diamond, the presence of the ^{13}C isotope (1.1 % natural abundance) introduces phonon scattering that limits its thermal conductivity. The scattering rate due to isotopic disorder scales with the mass variance $(\Delta M/M)^2$. This type of phonon scattering is known as:
   A. Mass-defect (isotope) scattering
   B. Phonon–electron scattering
   C. Phonon–phonon Umklapp scattering
   D. Grain-boundary (surface) scattering

10. (1 point) Creep is time-dependent deformation under constant stress. Primary creep exhibits:
    A. Increasing strain rate
    B. Decreasing strain rate
    C. Constant strain rate
    D. Rapid failure

11. (1 point) Flexural strength (modulus of rupture) is determined from a three-point bend test by:
    A. Maximum tensile stress at fracture
    B. Maximum compressive stress at fracture
    C. Maximum shear stress at mid-span
    D. Average stress across section

12. (1 point) In tungsten carbide (WC), the thermal expansion coefficient is $\alpha = 5 \times 10^{-6}\,\mathrm{K}^{-1}$, whereas for cobalt binder $\alpha = 13 \times 10^{-6}\,\mathrm{K}^{-1}$. Under rapid heating, this mismatch causes:
    A. Compressive stress in WC
    B. Tensile stress in WC
    C. No stress
    D. Shear failure only

13. (1 point) The Guinier approximation in small-angle X-ray scattering is valid for $qR_g < 1$, where $q = 4\pi \sin\theta/\lambda$ and R_g is the radius of gyration. It predicts $\ln I(q) \propto -q^2 R_g^2/3$. This allows direct extraction of
    A. crystal size
    B. particle shape
    C. radius of gyration
    D. lattice parameter

14. (1 point) A powder XRD pattern of rock-salt NaCl is collected with Cu Ka radation. Which Miller indices respond to the 5th diffraction line?
    A. (220)

B. (222)

C. (210)

D. (211)

15. (1 point) A compound with $r_{cat}/r_{an} \approx 0.800$ is most likely to adopt which coordination geometry?

A. Linear

B. Tetrahedral

C. Octahedral

D. Cubic

16. (1 point) Kikuchi lines in TEM diffraction arise primarily from

A. elastic Bragg scattering

B. inelastic diffraction of thermal diffuse scattering

C. fluorescent X-rays

D. electron–electron scattering

17. (1 point) The "phase problem" in crystallography refers to the inability to measure directly the

A. structure-factor amplitudes

B. structure-factor phases

C. unit-cell dimensions

D. Bragg angles

18. (1 point) In semiconductor doped Si, vacancy concentration under n-type doping:

A. Increases

B. Decreases

C. Unchanged

D. Oscillates

19. (1 point) The Kirkendall effect demonstrates:

A. Vacancy flow markers

B. Dislocation motion

C. Grain boundary migration

D. Precipitate growth

20. (1 point) A key advantage of powder diffraction over single-crystal methods is that

A. it requires no single crystal

B. it gives directional intensities

C. it solves phases directly

D. it has no peak overlap

21. (1 point) Given that the pressure is constant, how many degrees of freedom does the α phase of Cu-Zn alloy have?

A. 0

B. 1

C. 2

D. 3

22. (1 point) The Avrami equation describes which of the following phenomena?
    A. The rate of atomic diffusion in a crystal lattice during steady-state diffusion
    B. The kinetics of phase transformation involving nucleation and growth
    C. The dependence of recrystallization temperature on strain rate
    D. The time-dependent dislocation density in cold-worked metals

23. (1 point) Why does adding oxides like CaO, Y_2O_3 or MgO to zirconia (ZrO_2) increase its stability and strength?
    A. Because Ca^{2+} ions replace some Zr^{4+} ions, introducing oxygen vacancies and stabilizing the cubic and tetragonal phases, which minimize crack formation and improve toughness
    B. Because CaO increases the grain boundary area, which impedes dislocation motion and strengthens the ceramic
    C. Because CaO reduces the thermal conductivity of ZrO_2 allowing it to retain heat and resist fracture
    D. Because CaO reacts with ZrO_2 to form an intermediate compound such as $CaZr_4O_9$, which has higher melting point and hardness

24. (1 point) A supersaturated $NaCH_3COO$ solution remains metastable until a seed crystal is added, at which point rapid precipitation occurs. Which of the following best explains why adding a seed crystal triggers instantaneous crystallization?
    A. The seed crystal increases the volumetric free energy change ΔG_v, lowering ΔG^*
    B. The seed crystal eliminates the surface area term in ΔG^*, making $\Delta G^* = 0$ and allowing spontaneous crystallization
    C. The seed crystal decreases the latent heat of crystallization, making the process exothermic and instantaneous
    D. The seed crystal reduces the effective interfacial energy γ thereby lowering ΔG^*

25. (1 point) According to Pauling's rules, which conformation of tetrahedra is most stable in ionic crystals?
    A. Edge-sharing tetrahedra
    B. Face-sharing tetrahedra
    C. Corner-sharing tetrahedra
    D. Isolated tetrahedra with no sharing

26. (1 point) Which of the following statements about the Fermi velocity (v_F) in metals is correct?
    A. It is the average drift velocity of electrons when a current flows through the metal
    B. It is the velocity of electrons at the Fermi energy at absolute zero temperature
    C. It is the speed of sound in the metallic lattice
    D. It represents the velocity at which all electrons move randomly inside the metal

2 Nucleation of ZnO Nanoparticles (20 points)

27. (15 points) A chemist is synthesizing ZnO nanoparticles by homogeneous nucleation in solution at $T = 298$ K. For one recipe, the effective interfacial energy is $\gamma_1 = 0.50\ \mathrm{J \cdot m^{-2}}$ without any capping agents. The effective γ drops to $\gamma_2 = 0.20\ \mathrm{J \cdot m^{-2}}$. The driving free energy density from supersaturation is $\Delta G_v = -1.0 \times 10^9\ \mathrm{J \cdot m^{-3}}$ which is consistent for both cases.

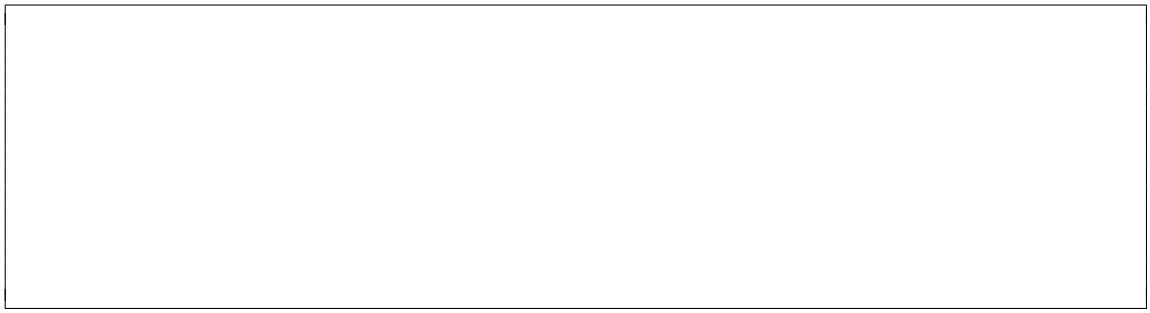
(a) For spherical nuclei, write the change in free energy ΔG as the function of nucleus radius r where $\Delta G_v < 0$ is the volume free energy per unit volume driving the phase change and γ is the interfacial energy between the nucleus and surrounding solvent.

(b) Derive expressions for the critical radius r^* and the nucleation barrier ΔG^*.

(c) Calculate r^* and ΔG^* for γ_1 and γ_2. Show numeric values in nm for radius and in joules for energy.

(d) Let the nucleation rates per unit volume are J_1 and J_2 for γ_1 and γ_2, respectively. The prefactor J_0 is identical in both cases. Compute the ratio $\frac{J_2}{J_1}$.

(e) Give physical and chemical mechanisms how capping agents or solvents lower γ.



3 An "Electrifying" Problem (15 points)

Your team is building a battery-powered "smart doorknob." When a (very small) touch current can flow through a metal-silicon contact, the lock wakes up; otherwise it sleeps to save power. You can choose the contact metal. The silicon handle is a single crystal wafer bonded inside the knob. Unless stated otherwise, assume the crystal to be silicon with a band gap of $E_g \approx 1.12eV$ and electron affinity $\chi \approx 4.05eV$, room temperature $300K$. You are offered three sputtered metals and given their work functions ϕ_M: aluminum ($\phi_M = 4.1eV$), titanium ($\phi_M \approx 4.3eV$), nickel ($\phi_M \approx 5.1eV$). The silicon can be doped either n-type (N_D) or p-type (N_A) at levels you request.

28. (6 points) For lightly doped n-Si ($N_D \sim 10^{16}cm^{-3}$), decide for each metal (Al, Ti, Ni) whether the metal-Si contact will behave more like a one-way gate (rectifying) or a free highway (nearly ohmic) at small forward biases. Justify using band-edge alignment ideas: think about where the metal Fermi level would sit relative to the semiconductor bands at the surface, and what that does to the electron flow from Si into the metal. Repeat the same reasoning for lightly doped p-Si with the same metals; explain any "role reversal" you predict.

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29. (4 points) On a hot summer day, the doorknob on the sun-facing porch starts waking the lock more often than in spring, with the exact same touch. Assume the metal and doping are such that the room-temperature contact was a one-way gate on n-Si. As the temperature rises, does the height of the energy barrier at the interface intrinsically increase, decrease, or stay constant? What does the change that explains the increased current?

30. (5 points) Your team now wants the doorknob sensor to work reliably in the cold outdoors. You use a Ti contact on n-type silicon with donor concentration $N_D = 5.0 \times 10^{17} cm^{-3}$. Assume the effective density of states in the conduction band $N_C = 2.8 \times 10^{19} cm^{-3}$. Take the temperature to be 250K. Determine the position of the Fermi level relative to the conduction band edge in bulk n-Si ($E_C - E_F$) at 250K. From this, calculate the built-in potential V_{bi} inside the silicon at equilibrium. Based on your numbers, explain in words whether you expect this Ti/n-Si contact to behave more like a "tunnel-ready bridge" (low-resistance/ohmic) or a "blocking barrier" (rectifying). Be explicit about why the values you computed lead you to this conclusion.

4 Quantum Dots (20 points)

31. (5 points) Quantum dots (QDs) are semiconductor nanostructures that confine charge carriers in all three spatial dimensions, creating discrete, atom-like energy levels.

    (a) Consider a cubic quantum dot with side lenght L. Electrons behave like free particles confined in a 3D infinite square well. When an electron-hole pair forms inside the quantum dot, they bind into an excition; the energy of an exciton can be approximated as

    $$E_{exciton} = E_e + E_h - \Delta$$

    where E_e is the electron's confinement energy, E_h is the hole's confinement energy, and Δ is the binding energy due to Coulomb attraction. Suppose the effective mass of the electron is $m^* = 0.067m_e$, and $L = 5nm$. If a hole has effective mass $m_h^* = 0.5m_e$, compute its ground-state confinement energy using the same formula as for electrons. Express in multiples of the E_0, where we take as given the 3D infinite-well result $E_{n_x,n_y,n_z} = E_0(n_x^2 + n_y^2 + n_z^2)$.

    (b) If $\Delta = 40meV$, find the exciton ground state energy in eV.

32. (2 points) Consider two identical quantum dots placed close enough that electrons can tunnel between them. In a (simplified) tight-binding model,[1] the Hamiltonian matrix for the electron states can be written as

    $$H = \begin{bmatrix} E_0 & -t \\ -t & E_0 \end{bmatrix}$$

    where $t > 0$ is the tunneling amplitude. Calculate the energy splitting between the bonding and anti-bonding states in terms of E_0 and t.

[1] The tight-binding model is an approach to the calculation of electronic band structure using an approximate set of wave-functions based upon superposition of isolated atomic wavefunctions; this is closely related to the LCAO method in chemistry.

33. (3 points) Suppose we can represent exciton creation in a basis of two quantum dots A and B. The basis states are: $|1,0\rangle, |0,1\rangle, |1,1\rangle$ corresponding to one exciton in dot A, one in dot B, and one in each. The Hamiltonian in this basis is

$$H = \begin{bmatrix} E_x & -J & 0 \\ -J & E_x & 0 \\ 0 & 0 & 2E_x + u \end{bmatrix}$$

where E_x is the single exciton energy, J is the inter-dot coupling, and U is an interaction penalty for having two excitons simultaneously. If $E_x = 1.5eV$, $J = 50meV$, and $U = 200meV$, compute the full set of energies for this system.

34. (3 points) Quantum dots exhibit size-tunable optical properties because electron and hole confinement shifts the effective band gap. This is exploited in QD-LED displays and biomedical tagging. An example of a substance that can be manufactured as a nanoparticle and exhibit quantum confinement is cadmium selenide (CdSe). CdSe has bulk band gap $E_g = 1.74eV$, $m_e^* = 0.13m_e$, $m_h^* = 0.45m_e$. Take $L = 4.0nm$, $\Delta = 0.050eV$. Compute ground-state emission energy and wavelength; if visible light spans 400-700nm, identify which transitions fall in the visible range.

35. (5 points) Now consider three quantum dots placed in a line, each with the same size $L = 4.0nm$. In a tight-binding approximation, their emission states hybridize; the Hamiltonian is

$$H = \begin{bmatrix} E_0 & -J & 0 \\ -J & E_0 & -J \\ 0 & -J & E_0 \end{bmatrix}$$

(a) (3 points) Using your ground state energy from the last question E_0, and $J = 40meV$, compute the three hybridized energies.

(b) (2 points) Explain qualitatively how such a coupling could broaden the emission spectrum in real QD arrays.

36. (5 points) Address the following.

(a) (2 points) For cubic confinement, argue why ground-state exciton is optically allowed for all polarizations.

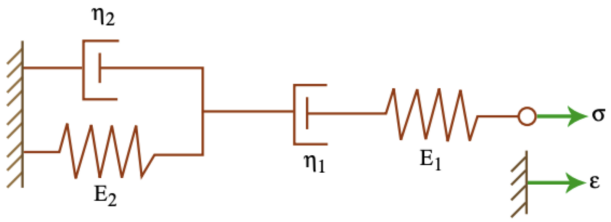
(b) (3 points) For excited states, explain why anisotropy leads to polarization-dependent absorption/emission.

5 Creep (15 points)

In addition to predicting the mechanical responses of linear viscoelastic materials like amorphous polymers, springs and dashpots can be used to created models of creep and recovery in crystalline materials. (Reminder: A spring creates a force proportional to displacement, and a dashpot dampens a system by creating a force proportional to velocity, in the opposite direction of velocity. These are ubiquitous in modeling mechanical behaviors in engineering.)

37. (4 points) Although springs and dashpots are used to predict the behavior of amorphous polymers and crystalline materials in response to mechanical loading, they are predicting two very different ways of dissipating mechanical energy. Explain the difference, precisely but concisely, in terms of elasticity, plasticity, and atomic/molecular mechanisms.

38. (4 points) Below is a model that accurately captures the creep and recovery response of several microcrystalline materials. For the given model, describe qualitatively how the strain in the microcrystalline material evolves over time under a step-stress applied at $t = 0$ and removed after a long time $t = t_1 >> 0$. In particular, explain the roles of each element (E_1, E_2, η_1, η_2) in the creep and recovery response.



39. (2 points) Returning to viscoelastic materials, the two simplest common models of describing stress and strain for such materials are the Kelvin-Voigt model and the Maxwell model. The Kelvin-Voigt model consists of one dashpot in parallel with one spring, while the Maxwell model consists of one dashpot in series with one spring. Give one advantage and one limitation of each model.

40. (5 points) Consider a Kelvin-Voigt material (elastic modulus E, viscosity η), subject to a harmonic strain $\epsilon(t) = \epsilon_0 \sin(\omega t)$. Derive an expression for the average dissipated power per unit volume (rate of energy dissipated as heat). (Hint: Write $\epsilon(t) = \epsilon_0 e^{i\omega t}$ and solve for the complex (dynamic) modulus $E^*(\omega) = \frac{\sigma(t)}{\epsilon(t)}$. The imaginary part E'' of $E^*(\omega)$ is the loss modulus; the energy dissipated per unit volume in one cycle is the area of the stress-strain hysteresis loop $W_d = \oint \sigma d\epsilon = \pi E'' \epsilon_0^2$)

6 Astro Marathon (20 points)

A team of space-people (?!) has shrunk down to the nanometer scale to investigate a new futuristic material called Hongjinium, a nanomaterial designed for spacecraft heat shields. Hongjinium forms a 2D crystalline sheet. A single sheet has dimension $1\mu m \times 1\mu m$ and its thickness is $1nm$.

41. (2 points) Calculate the surface area-to-volume ratio (SA/V) of this sheet in units of nm^{-1}. Briefly explain why this high SA/V ratio is beneficial for heat dissipation in a spacecraft heat shield.

42. (2 points) Two scientists debate how Hongjinium was made. Johnny says it was milled and etched down from a bulk crystal. Alex says it was built atom-by-atom using chemical vapor decomposition. Identify which scientist describes a top-down method and which describes a bottom-up method. Who's more likely correct, and why?

43. (5 points) The space-people bring out their instruments, and observe the following:

- X-ray diffraction: Sharp peaks observed
- Transmission electron microscopy: Reveals thin sheet-like patterns
- Energy dispersive spectroscopy: Confirms presence of embedded metal atoms

What does each technique reveal about Hongjinium? Together, how do these results confirm its 2D crystalline structure with metal atoms?

44. (3 points) They observe 90% absorption of visible light at 500nm wavelength. Give 3 reasons for why strong absorption of visible light might occur in such a nanomaterial?

45. (2 points) Hongjinium has a thermal conductivity of $2000 W/m \cdot K$, while typical stainless steel only has $15 W/m \cdot K$. Explain how this extraordinary thermal conductivity would protect a spacecraft during re-entry.

46. (3 points) At low temperatures and in very clean crystals, heat can travel as a wave rather than by ordinary diffusion. This phenomenon—second sound—arises when quantized lattice vibrations (phonons) behave collectively like a fluid. In the lab, the spacepeople can cool Hongjinium and excite it with a pulsed laser to watch how heat moves in the 2D sheet. For a 2D crystalline sheet like Hongjinium, list two material or environmental conditions that would favor observing second sound. Briefly justify each in terms of phonon behavior.

47. (3 points) Hongjinium contains embedded metal atoms in its lattice. Predict whether these inclusions are more likely to promote or suppress second sound, and explain your reasoning using quantum mechanical ideas about phonon scattering.