Name _____

MBSE Core Competency Exam

Wednesday, June 5, 2024 10:00 am – 1:00 pm

Instructions:

- You have three hours in which to complete the exam.
- Answer all four questions they all carry the same weight, and they all require approximately the same effort and length of answer. Note that the questions are arranged so that each appears on a separate page.
- Be sure to read each question carefully, and please ask for clarification if you don't understand the meaning.
- Please start your answer to each question on a new page.
- Include all the details of your thought process, along with any sketches, graphs, equations, and derivations needed to support your arguments. Be sure to label all sketches and graphs clearly, define all variables that you use, and clearly state all relevant assumptions.
- Your answers must contain only your own work. You may not consult any outside sources (written, spoken, or electronic) during the exam.
- You will find some potentially useful tables at the end of this document.

Good luck!

Bonding-structure-property relationships.

Part A

- (a) If you are tasked to select a material for cutting sapphire, what material would you choose? Explain your reasoning.
- (b) Now you are asked to cut steel. Would you still use the same material selection in (a) for the cutting blade? If not, what material would you choose? Explain your reasoning.
- (c) In order to lower cost, you are asked to design a transition metal-based ceramic for cutting tool applications. Please describe your design principles and your reasoning.
 Hint: Materials that can be effective in cutting structural materials require high hardness, high incompressibility, and good thermal stability.
- (d) You are getting bored and tired of working on ultra-hard and ultra-incompressible materials after spending years researching them. Just for fun, you want to "play" with metals that are so soft that you can cut them with a kitchen knife. What metals would have such properties? Explain your reasoning.

Part B

You are interviewing for a job in a battery company. One of their priorities is to develop *inorganic* solid-state *ion* conductors that can replace liquid electrolytes. Through conversations, it became obvious that, if you can propose strategies to realize that goal, you have a good chance of getting the job. Using the knowledge of crystal structures that you have learned in MBSE 210, please describe some ideas you can pitch to the company.

Hint: Think in terms of the characteristics of different crystal structures and the properties that would enable a solidstate compound to conduct ions efficiently.

Structure, physical properties.

Restingtonite is a polymorphic mineral; its crystal structure is tetragonal below 63.1°C (α -polymorph) and orthorhombic at 63.1°C and above (β -polymorph). Both polymorphs are optically transparent. Thin wafers prepared from single crystals are being evaluated as possible substrates for optoelectronic devices.

- (a) If the in-plane thermal expansion coefficient of these substrates is to be isotropic at temperatures in the range 50°C to 60°C, what should the orientation of the wafers be relative to the crystal axes of the α -polymorph? You may specify "orientation" in terms of the angles between the crystal axes and the normal to the wafer.
- (b) What can you predict about the optical behavior of the substrates prepared in (a) when they are observed at temperatures in the range 50°C to 60°C between crossed linear polarizers?
- (c) If the substrates prepared in (a) are used at temperatures in the range 70°C to 80°C, would their in-plane thermal expansion coefficient remain isotropic? Explain your answer carefully.
- (d) If the substrates prepared in (a) are characterized at temperatures in the range 70°C to 80°C, what can you predict about their optical behavior when they are observed between crossed linear polarizers?
- (e) To guarantee that substrates used at temperatures in the range 70°C to 80°C exhibit isotropic in-plane thermal expansion at those temperatures, what should the orientation of the wafers be relative to the crystal axes of the β -polymorph? The principal thermal expansion coefficients of the β -polymorph are 1.5×10^{-6} K⁻¹, 1.8×10^{-6} K⁻¹ and 2.4×10^{-6} K⁻¹ along axes designated X_1 , X_2 and X_3 respectively.
- (f) Under what circumstances would the substrates prepared in (e) be optically isotropic?

Thermodynamics, stability.

The molar Gibbs free energy \hat{G} of a uniform binary solution at some fixed temperature *T* and pressure *P* may have a dependence on the mole fraction *x* of one of the components that looks qualitatively like this:



- (a) In light of the curve, explain qualitatively but in some detail the reasons why such a solution might be stable, metastable, or spontaneously unstable under these conditions. As (a small) part of your explanation, be sure to address the basic meaning of the notion of stability under the specified conditions.
- (b) In light of your explanation, identify quantitative criteria for defining the boundaries between composition ranges in which the solution is stable, metastable, and unstable, and sketch those boundaries relative to the curve.
- (c) Show how to obtain from the graph the chemical potentials of the two species for all compositions x (i.e., the entire domain $x \in [0, 1]$) at the temperature and pressure corresponding to the curve.
- (d) Explain how to obtain the phase compositions in all phase-separated states. Use a sketch to define clearly and unambiguously any values needed in your method.
- (e) Explain how to obtain the phase fractions in all phase-separated states. Write down explicit formulas for them, and use a sketch to define clearly and unambiguously any values needed as input.
- (f) How (and why) would the curve change if the temperature is increased and if it is decreased?
- (g) Sketch a qualitatively reasonable representation of the temperature-composition (T-x) phase diagram at the fixed pressure *P*, and label clearly the significant regions and points. On your diagram, indicate the temperature corresponding to the \hat{G} curve above.
- (h) In light of your phase diagram, explain in some detail what happens in the system when *T* starts out at a high (relative to any features on your phase diagram) value and heat is removed at a constant rate that is slow enough to keep the system in equilibrium.

Mechanical properties.

- (a) During the course of your MBSE studies, you have encountered multiple ways to quantify the "strength" of a material subjected to tensile loads. They include (i) proof strength, (ii) elastic limit, (iii) proportional limit, (iv) offset yield strength, (v) ultimate tensile strength, (vi) breaking strength, and (vii) the quantity σ_0 in the Weibull distribution of failure probability. Carefully describe how each of these parameters is defined and properly interpreted.
- (b) How does microstructure affect the measures of "strength" listed in (a)?
- (c) Some of the above measures of "strength" can be expressed as both "nominal" and "true" values. How are "nominal" and "true" defined, and which of the measures of "strength" listed in (a) can be expressed in both ways? Why can't all the measures of "strength" listed in (a) be expressed in both ways?

		Viewing	g directio	ns	Point group /		
system	defining symmetry	I st letter	2 nd letter	3 rd letter	crystal class (full symbol)		
Triclinic	1-fold symmetry	l or $\overline{1}$			l or 1		
Monoclinic	One 2-fold (diad)	b (c)			2, m, $\frac{2}{m}$		
Orthorhombic	Three 2-folds (diad)	а	b	С	222, 2mm, $\frac{2}{m} \frac{2}{m} \frac{2}{m} \frac{2}{m}$		
Tetragonal	One 4-fold (tetrad)	С	а	[110]	4, $\overline{4}$, $\frac{4}{m}$ 422, 4mm, $\overline{4}2m$, $\frac{4}{m}\frac{2}{m}\frac{2}{m}$		
Trigonal	One 3-fold (triad)	С	а	[210]	3, $\overline{3}$ 32, 3m, $\overline{3}\frac{2}{m}$		
Hexagonal	One 6-fold (hexad)	С	а	[210]	6, $\overline{6}$, $\frac{6}{m}$ 622, 6mm, $\overline{6}2m$, $\frac{6}{m}\frac{2}{m}\frac{2}{m}$		
Cubic	Four 3-folds (triad)	а	[111]	[110]	$23, \frac{2}{m}\overline{3} \\ 432, \overline{4}3m, \frac{4}{m}\overline{3}\frac{2}{m}$		

Useful Information

Periodic Table of Elements																	
1 H 1.00794																	He 4.002602
3 Li 6.941	4 Be 9.012182											5 B 10.811	C 12.0107	7 N 14.00674	8 0 15.9994	9 F 18.9984032	10 Ne 20.1797
11 Na 22.989770	12 Mg 24.3050											13 Al 26.581538	14 Si 28.0855	15 P 30.973761	16 S 32.066	17 Cl 35.4527	18 Ar ^{39.948}
19 K 39.0983	20 Ca 40.078	21 Sc 44.955910	22 Ti ^{47.867}	23 V 50.9415	24 Cr ^{51.9961}	25 Mn 54.938049	26 Fe 55.845	27 Co 58.933200	28 Ni ^{58.6534}	29 Cu 63.545	30 Zn 65.39	31 Ga 69.723	32 Ge 72.61	33 As 74.92160	34 Se _{78.96}	35 Br 79.504	36 Kr ^{83.80}
37 Rb 85.4678	38 Sr 87.62	39 Y 88.90585	40 Zr ^{91.224}	41 Nb 92.90638	42 Mo _{95.94}	43 Tc (98)	44 Ru 101.07	45 Rh 102.90550	46 Pd 106.42	47 Ag 196.56655	48 Cd 112.411	49 In 114.818	50 Sn 118.710	51 Sb 121.760	52 Te 127.60	53 126.90447	54 Xe 131.29
55 CS 132.90545	56 Ba 137.327	57 La 138.9055	72 Hf 178.49	73 Ta 180.94.79	74 W 183.84	75 Re 186.207	76 Os 190.23	77 Ir 192.217	78 Pt 195.078	79 Au 196.56655	80 Hg 200.59	81 TI 204.3833	82 Pb 207.2	83 Bi 208.58038	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	89 Ac (227)	104 Rf (261)	105 Db (262)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (266)	(269)	(272)	(277)		114 (289) (287)		(289)		(293)

58	59	60	61	62	63	64	65	66	67	68	69	70	71
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
140.116	140.50765	144.24	(145)	150.36	151.964	157.25	158.92534	162.50	164.93032	167.26	168.93421	173.04	174.967
90	91	92	93	94	95	96	97	98	99	100	101	102	103
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
232.0381	231.035888	238.0289	(237)	(244)	(243)	(247)	(247)	(251)	(252)	(257)	(258)	(259)	(262)