MBSE Core knowledge exam

Wednesday, June 2, 2021 **Name** ____________________

Instructions: You have three hours to complete the exam. Answer all of the questions—they all carry the same weight.

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 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, including calculators) during the exam.

You'll find some potentially useful tables at the end.

Good luck!

1. ***Critical sizes.*** Consider the following two situations:

i. An embryo forms spontaneously in molten copper, below the equilibrium temperature for solidification.
ii. A crack grows slowly in a large piece of mild steel.

Once the embryo reaches a critical dimension (the critical nucleus size), continued growth under the prevailing conditions is assured. Similarly, once the crack reaches a critical dimension (the critical crack length), continued growth under the prevailing conditions is assured.

Demonstrate how, in both cases, a simple energy balance can be used to derive the critical dimension in terms of appropriate material properties.

2. *Origins of properties.*

(a) With reference to reciprocal space (k-space), explain how electron energy bands and band gaps arise in solids. What are the significance of Brillouin zones and the Fermi surface in this context? How do these concepts relate to the properties of real materials?

(b) ScN and TiN both adopt the rock salt structure. ScN is an electrical insulator, whereas TiN is a good electrical conductor.

Please explain the reason behind the difference in electrical properties. Sketch diagrams to aid your explanation.

(c) Based on your answer from (b), what is the nature of the bonding in ScN vs. TiN?

(d) How would you describe the rock salt structure using the space-sharing polyhedra model?

3. ***Crystal symmetry.***

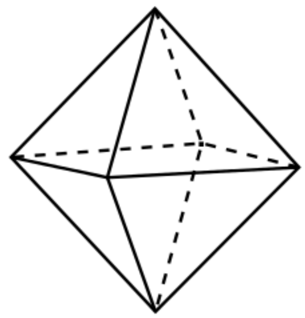
(a) What is the maximum number of non-zero, non-equal coefficients that are needed to describe the thermal expansion of

i. a triclinic crystal,
ii. an orthorhombic crystal,
iii. a hexagonal crystal, and
iv. a cubic crystal,

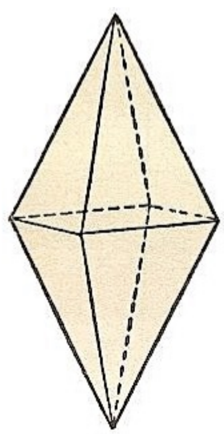
when in each case the temperature is changed by 5 °C from one uniform value to another. Clearly state your reasoning, along with any assumptions.

(b) Based on symmetry, to which crystal system do each of the following single crystals belong? Please explain your reasoning.

i. A regular octahedron:



ii. A shape like a regular octahedron that has been elongated uniformly in one direction, as shown:



4. ***The titanium-silicon system.***

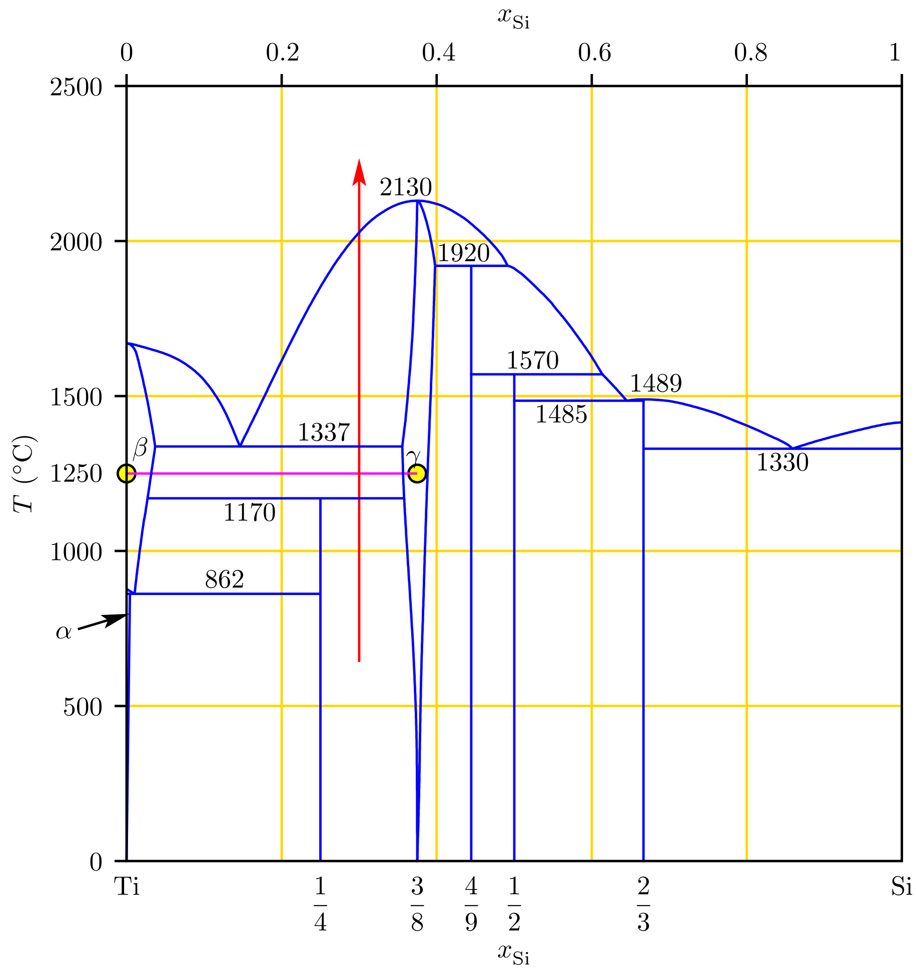


Figure 1: The temperature-composition phase diagram of the solid and liquid phases of the titanium-silicon system at 1 bar. The regions labeled α, β, and γ, and the straight vertical lines are single-phase regions, the latter having near-zero width. The α phase, occupying just a barely visible sliver on the diagram, has the hexagonal-close-packed (HCP) structure, the β phase has the body-centered-cubic (BCC) structure, and the γ phase has composition near that shown at the bottom of its range. The numeric labels inside the frame indicate the temperatures of the adjacent horizontal lines or peaks of the adjacent curves. Note that the horizontal line at 1250 °C, the vertical arrow at $x_{\mathrm{Si}} = 0.3$, and the temperature and composition grid lines are not features of the phase diagram.

Figure 1 shows a phase diagram for the titanium-silicon system.

(a) Sketch a qualitatively accurate set of molar Gibbs-free-energy curves $\widehat{G}(x)$ of all of the competing phases for $T = 500$ °C. Explain the logic behind your selection of phases and your choices of the positions and features of the curves.

(b) Describe in detail the progression of thermodynamic equilibrium states of the system along the red line at $x_{\mathrm{Si}} = 0.3$, from the bottom of the line to the tip of the arrow at the top. Don't neglect the details of any phase transitions that occur.

(c) Suppose we arrange somehow to maintain a constant source of pure Ti at the left end (position coordinate $x = 0$) of a long bar of Ti_5Si_3.

i. Sketch the concentration profiles of Ti and Si prior to any interdiffusion.

ii. Now suppose we raise and hold the temperature at 1250 °C, indicated in Figure 1 by a horizontal line with dots at its endpoints, the compositions of pure Ti and of the bar prior to any interdiffusion. Explain what happens subsequently.

iii. Sketch qualitatively the concentration profiles you would expect to measure after several hours and again after several more hours.

Periodic Table of Elements

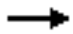
1 H 1.00794																	2 He 4.002602
3 Li 6.941	4 Be 9.012182											5 B 10.811	C 12.0107	7 N 14.00674	8 O 15.9994	9 F 18.9984032	10 Ne 20.1797
11 Na 22.989770	12 Mg 24.3050											13 Al 26.581538	14 Si 28.0855	15 P 30.973761	16 S 32.066	17 Cl 35.4527	18 Ar 39.948
19 K 39.0983	20 Ca 40.078	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 I 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 Tl 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)	110 (269)	111 (272)	112 (277)		114 (289) (287)		116 (289)		118 (293)

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

Table 1

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

Table 2

Symmetry Element	**Graphical Symbol**	**Translation**	**Symbol**
Identity	None	None	1
2-fold ⊥ page		None	2
2-fold in page		None	2
2 sub 1 ⊥ page		1/2	2_1
2 sub 1 in page		1/2	2_1
3-fold		None	3
3 sub 1		1/3	3_1
3 sub 2		2/3	3_2
4-fold		None	4
4 sub 1		1/4	4_1
4 sub 2		1/2	4_2
4 sub 3		3/4	4_3
6-fold		None	6
6 sub 1		1/6	6_1
6 sub 2		1/3	6_2
6 sub 3		1/2	6_3
6 sub 4		2/3	6_4
6 sub 5		5/6	6_5
Inversion		None	1
3 bar		None	3
4 bar		None	4
6 bar		None	$6 = 3/m$
2-fold and inversion		None	$2/m$

2 sub 1 and inversion		None	$2_1/m$
4-fold and inversion		None	$4/m$
4 sub 2 and inversion		None	$4_2/m$
6-fold and inversion		None	$6/m$
6 sub 3 and inversion		None	$6_3/m$

Table 3

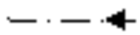
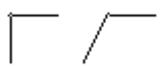
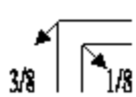
Symmetry plane	Graphical symbol	Translation	Symbol
Reflection plane		None	*m*
Glide plane		1/2 along line	*a*, *b*, or *c*
Glide plane		1/2 normal to plane	*a*, *b*, or *c*
Double glide plane		1/2 along line & 1/2 normal to plane	*e*
Diagonal glide plane		1/2 along line & 1/2 normal to plane	*n*
Diamond glide plane		1/4 along line & 1/4 normal to plane	*d*

Table 4

Symmetry plane	Graphical symbol	Translation	Symbol
Reflection plane		None	*m*
Glide plane		1/2 along arrow	*a*, *b*, or *c*
Double glide plane		1/2 along either arrow	*e*
Diagonal glide plane		1/2 along the arrow	*n*
Diamond glide plane		1/8 or 3/8 along the arrows	*d*