Advanced Tutorial in Materials Science and Engineering (2)

Summer 2015: Intensive Lectures (5 weeks : June 17-July 24) At Tohoku University, Sendai, Japan

Course Objective: この集中講義は 私が現在ワシントン大学工学部物質材料学科で行っている物質材料科学総論(学部高学年及び大学院初年度学生向け)をもとにして作られたものです。 物質材料科学は今や理工各分野に浸透しそれぞれユニークな発展をとげていることは周知の通りですが、それだけに物質材料科学全体をもう一度レビューしてみよう、または専攻は違っても自分なりの物質材料科学を構築してみようと思う学生諸君にこの集中講義は役に立つと思います。講義は英語で行いますが、言葉の壁を乗り越えて学生諸君と授業での交流を大切にします。私は26歳で渡米し今年でアメリカ在住40年になりましたが、 今までの私の経験が皆さんのなにかに役に立てればと思いこの集中講義を行います。奮って参加してください。

This is an advanced tutorial of Materials Science and Engineering at the senior and/or entrygraduate levels. The course is specifically designed for those who did not major in the field of Materials Science and Engineering (MSE) as undergraduates, yet whose research is closely related to MSE discipline, and/or those who wish to re-examine their knowledge of Materials Science and Engineering from a broader perspective. This course will focus on the nature of materials' physical and chemical structures, and their relationship to mechanical, electrical, dielectric, optical, magnetic and thermal properties. Emphasis will be on modern thinking about the materials principles and practice together with their structure-property-performance relationship in a form that is readily accessible to students in all disciplines.

Instructor:	Professor Fumio S. Ohuchi Department of Materials Science and Engineering University of Washington Seattle, WA 98195, USA ohuchi@u.washington.edu (206) 685-8272
Lectures:	 4:20-5:50PM 3 times/week for 5 weeks (Monday, Wednesday and Friday) Note: • First class on Wednesday, June 17, 2015. • July 22(W)-lecture will be held on July 21(Tues). • Last class on Friday, July 24, 2015. • Tentative schedule sheet is attached.

Course Contents:

Lecture material samples (selected from the Lecture Note) are attached for your information.

- [I] What's Unique About Materials Science & Engineering?
 - Thermodynamically versus kinetically controlled process and phenomena
 - Imperfections in solids: Thermodynamics legitimate questions
 - Driving forces of the material process

[II] Materials With metallic bonding

- Electron energy states and metallic bonding: relation to the properties
- Group I, II, III and transition metals; how are the electrons distributed?
- Significance of the Fermi energy

- [III] An Atomic View of Materials
 - Energy and packing: order vs. disorder
 - Crystal structure and atomic packing
 - Basics (Review) of the crystallography
- [IV] Materials With Ionic & Covalent Bonding
 - · Ionic-covalent mixed bonding, and charge density
 - Madelung constants
 - Factor influencing the crystal structures
 - Imperfections in materials; Hume-Rothey rules
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 - What can you learn from the phase diagram?
 - Materials processing

[VI] Materials Under Mechanical Stress

- Stress-strain relationship
- Processes involved in the plastic deformation
- What causes "material's failure"?
- "Karate" as an example!

[VII] Electrical Conduction and Semiconductivity

- Visualization of electrical conduction in metals and semiconductors
- · Semiconductor surfaces and junction properties
- Basic devices: metal-sc junctions, p-n junctions and MOSFET

[VIII] Dielectric & Optical Properties of Materials

- Dielectric vs. optical: relationship through frequency
- Specific to the dielectric and optic
- Optical dispersion of materials
- · Absorption and recombination processes in semiconductors

Grading:	HW (self-grading) 5-times	10%
	Midterm exam (in-class) Final exam (in-class)	40% 50%
Pre-requisite:	No prerequisite is required prepare basic background by	to take this course, but the students are asked to y themselves.
Course pack:	Available in PDF files prove Lectures will follow the cou	ided in class rse pack.

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[1] WHAT'S UNIQUE ABOUT MATERIALS SCI. & ENG.?



The concept of **materials science tetrahedron (MST)** concisely depicts the inter-dependent relationship among the structure, properties, performance, and processing of a material.

We start with several examples to illustrate the subjects unique to MSE

- (1). *Thermodynamically* versus *Kinetically* controlled processes and phenomena in materials
- (2). *Kinetic rate equations* and *driving force(s)* in materials, and the rate equations.
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Driving Forces Governing various Phenomena

Rate of transformation: Rate= βF					
Process	Driving Force F	Typ. values (J/Mole)			
Fracture	$V_m \sigma^2/(2Y)$	0.5	σ: stress at failure Y: Young's modulus		
Grain growth	$2\gamma_{gb}/r$	20	γ_{gb} : grain boundary energy r: radius of a particle		
Sintering	2γ/r	100	γ: surface energy r: curvature		
Creep	σV_m	1000	σ : applied stress V_m : molar volume		
Crystallization	$\Delta H \Delta T / T_m$	3000	ΔH : enthalpy of transf. ΔT : under cooling		
Inter diffusion	$RT(x_a ln x_a + x_b ln x_b)$	5000	Ideal sulution		
Oxidation	ΔG_{form}	50,000- 500,000	Free energy of formation of oxide; a per-mole-of-O.		

Assumptions : 1000K, molar volume: 10⁻⁵m³/moll, r ~1μ, g=1J/m². σ=100MPa





Thermodynamics vs. Kinetics Example (5): Growth of Metastable phase



Kinetics versus Thermodynamics Process



Imperfections in Solids

- Properties profoundly influenced by the presence of imperfections.
- Knowledge about the types of imperfections that exist and the roles they play in affecting the behavior of materials.
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Atom Purity and Crystal Perfection

- There are no perfect crystals.
- Material properties are "improved" by the presence of imperfections and deliberately modified.

Why do we care about defects?

Examples

Mechanical properties: • Metal alloys for improving strength.

Electrical properties:

Control of conductivity and charge carrier mobilities.

Optical properties:

Wavelengths of light being absorbed and/or emitted by materials

Defects and Materials Technology Several Examples



Thermodynamics Legitimate Questions We know:

- To melt materials, we need heat. "Melting is endothermic".
- To form point defects, we need to remove atoms from solid (i.e. vacancy). "Breaking bond" is **endothermic**.

"Melting" and "Vacancy" occurs even it costs energy. WHY?

You may answer:

At the equilibrium, we must consider the **"free-energy"** rather than the **"enthalpy"**, then minimize the free-energy. The **"entropy"** changes associated with the formation of the melting and defect formation can reduce the free energy

of the "system", since G=H-TS, where H is always positive, so G could become negative at some T.

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MATERIALS WITH METALLIC BONDING

- · What promotes metallic bonding?
- What properties are inferred from metallic bonding?
- · Basis of the electronic structure of metals

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ble 2.1	The Number Shells and Sul	of Available bshells	Electron Stat	tes in Some of t	he Electron	Quantum #	Des	ignation
incipal	Shall		Number of	Number oj	<i>Electrons</i>	n = principal (energy leve	el-shell)	K, L, M, N, O (1, 2, 3, etc.)
umber n	Designation	Subshells	States	Per Subshell	Per Shell	1 = subsidiary (orbitals)		cndf(0100, n1)
	K	3	1	2	2	1 – subsidiary (orbitals)		s, p, u, j (0, 1, 2, 3,, n-1)
	,	5	1	2	0	$m_l = magnetic$	1, 3,	5, 7 (-l to +l)
	L	p	3	6	0	m – min	14	14
		8	1	2		$m_s = \text{spin}$	42, -	-72
	М	p	3	6	18			
		d	5	10				
		5	1	2				
	N	p	3	6	32			
		d	5	10				
		1	7	1.4				

SURVEY OF ELEMENTS

•	Most elements:	Electron configuration is not stat	bl	e.
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Element	Atomic #	Electron configuration		
Hydrogen	1	15 1		
Helium	2	1s 2 (stable)		
Lithium	3	15 225 1	15	
Beryllium	4	1S 22S 2		
Boron	5	18 228 22p 1	28 2p	Y X X X X
Carbon	6	18 228 22p 2	3s 3p 3d	
			to the till the	
Neon	10	18 228 22p 6 (stable)	45 40 40 41	
Sodium	11	1s 22s 22p 63s 1	58 5P 50 51 58	
Magnesium	12	1s 22s 22p 63s 2	6s 6n 6d 6f 6g	
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Group-I metals

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Rb : Sr Cs : Ba

This is why BCC is taken Group I vs

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Li : Be	45
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K : Ca	333

1s vs. 2s orbital

Secondary peak near the nucleus: e- penetrates fairly deeply in the atom from time to time. Similar way that Halley's comet nips quickly round the part of its orbit close to the sun (but takes 75 years). For 2s electron, it repeats about 2MM times every nano-seconds.

Group-II metals

Filled in s-orbital Crystallizes into a closed packed (CN#=12) Next nearest neighbours(CN#=6) occurs further off.

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	Melting Temp (K)
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Group II elements all have higher T_m . More rattle energy is needed to break their bonds, therefore stronger bonding.

Explore how properties change with temperature















A technique to solve this equation using this approximation is called:

Kronig-Penny potential model

- · Isolate valence electrons from core electrons
- Simplified potential shape
- Impose the lattice periodicity on the wave function



















Significance of the Fermi Energy (2) Thermionic Emission





Polarization effects on melting temperature











- · How do atoms assemble into solid structures?
- · How does the density of a material depend on its structure?
- When do material properties vary with the sample (i.e., part) orientation?
- The properties of some materials are directly related to their crystal structure.
 Significant property differences exist between crystalline and noncrystalline materials having the same composition.

Back ground	MSE 170 (Callister: Chapters 3, 12, 14)
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Energy and Packing: Order vs. Disorder



Dense, ordered packed structures tend to have lower energies.

Metallic Crystal Structures

- (1) Tend to be densely packed.
- (2) Reasons for dense packing:
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ATOMIC PACKING FACTORS BCC and FCC



DENSITIES OF MATERIAL CLASSES





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• There are four tetrahedral sites on each of the six BCC cell faces • You see total 4 x 6 = 24 tetrahedral voids • Each face V2 shared, so 24 x (1/2)=12 tetrahedral voids (sites) per cell • Tetrahedral voids in BCC are asymmetric



 You see 1+12=13 octahedral sites. Center = 1 Edge center 1/4 share = 12 x(1/4)=3
 So, total of 1+3=4 octahedral voids (sites) per FCC cell
 Center octahedral void in FCC is symmetric
 Edge center octahedral voids are asymmetric



Located at {1/4,1/4,1/4} - center of cell octet
 There are 8 tetrahedral voids per FCC cell
 All are symmetric

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Suggested reference books for background information: Any of the following comprehensive text books introducing Materials Science and Engineering will serve as the reference for background.

- William D Callister, Jr. and David G. Rethwisch, <u>Materials Science and Engineering</u>: <u>An Introduction</u>, 6, 7 or 8th Editions, Wiley.
- James F. Shackelford, Introduction to Materials Science for Engineers, 6 or 7th Edition, Macmillan.
- Donal R. Askeland and Pradeep P. Phule, <u>The Science and Engineering of Materials</u>, 5th/6th Edition, Thomson.
- L. H. Van Vlack, Elements of Materials Science and Engineering, 6th Edition,
- Craig R. Barret, William D. Nix and Alan S. Teleman, <u>The Principles of Engineering Materials</u>, Prentice-Hall, Inc. (classical book)
- Charles A. Wert and Robb M. Thomson, <u>Physics of Solids</u>, McGraw-Hill, 2nd edition (classic book)

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	K	3	1	2	2	I = subsidiary (orbitals)		s, p, u, j (0, 1, 2, 3,, n-1)
	,	5	1	2	0	$m_l = magnetic$	1, 3,	5, 7 (-l to +l)
	L	p	3	6	0	m – min	14	14
		8	1	2		$m_s = \text{spin}$	72,-	-72
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٠	Most elen	ients: El	ectron	configurat	tion i	s not	stal	ole.
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			as an ad af	
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Group-I metals

Half filled in s-orbital Crystallizes into a BCC structure 8 nuclei as nearest neighbours (CN#=8) and another second nearest (CN#6) only 15 % further away.

Cs : Ba

This is why BCC is taken Group I vs

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- The electron cloud sinelds cores from each other



ATOMIC PACKING FACTORS BCC and FCC



DENSITIES OF MATERIAL CLASSES





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• There are four tetrahedral sites on each of the six BCC cell faces • You see total 4 x 6 = 24 tetrahedral voids • Each face V2 shared, so 24 x (1/2)=12 tetrahedral voids (sites) per cell • Tetrahedral voids in BCC are asymmetric



 You see 1+12=13 octahedral sites. Center = 1 Edge center ¼ share = 12 x(1/4)=3 So, total of 1+3=4 octahedral voids (sites) per FCC cell Center octahedral void in FCC is symmetric Edge center octahedral voids are asymmetric



Located at {1/4,1/4,1/4} - center of cell octet
 There are 8 tetrahedral voids per FCC cell
 All are symmetric
 6