

PY2N20

**Material Properties and
Phase Diagrams**

Lecture 1

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Text Books

- *Materials Science & Engineering
An Introduction*
William D Callister, Jr.
S-LEN 620.11 53*5;1 10
- *Introduction to Materials Science for
Engineers*
James F Shackelford
620.11 M56*5

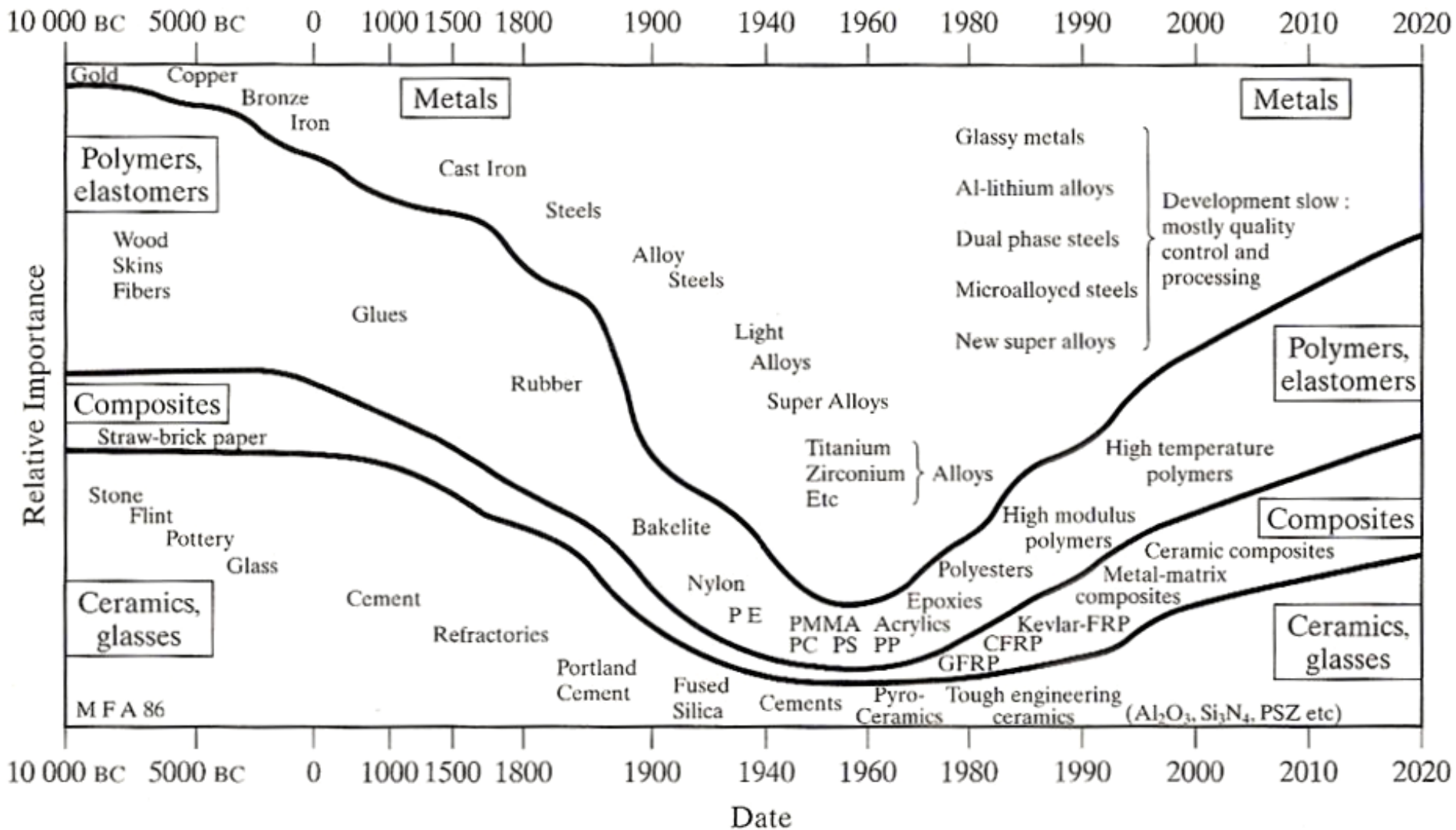
Handouts, Notes, Tutorials, etc.

- Handouts will be distributed at each of the lectures
- After the lectures electronic copies of the corresponding handouts will be uploaded at:

<http://physics.tcd.ie/people/Plamen.Stamenov/Courses/>

- The examination questions are already fixed
- Voluntary tutorials to be organised...

Historical Perspective



- Metals, Polymers, Composites, Ceramics, Glasses

Types of Materials

- Metals
- Ceramics
- Semiconductors
- Polymers
- Composites

Metals

IA 1 H	II A 4 Be											III A 5 B	IVA 6 C	V A 7 N	VIA 8 O	VIIA 9 F	O 2 He
3 Li	11 Na											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg												

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lw

- Most elemental compounds are metals – rules of QM!

Ceramics

IA																		O
1	II A											III A	IVA	VA	VIA	VII A		2
H	Be											B	C	N	O	F		He
3	4											5	6	7	8	9		10
Li	Be											B	C	N	O	F		Ne
11	12											13	14	15	16	17		18
Na	Mg	III B	IV B	V B	VII B	VIII					IB	II B	Al	Si	P	S	Cl	Ar
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35		36
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br		Kr
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53		54
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I		Xe
55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85		86
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At		Rn
87	88	89	104	105	106													
Fr	Ra	Ac	Rf	Db	Sg													

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
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	Lw

- Based on oxides, sulphides, nitrides, but not only!

Semiconductors

I A																		O
1 H	II A												III A	IVA	VA	VIA	VIIA	2 He
3 Li	4 Be												5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg	III B	IV B	V B	VIB	VII B	VIII				IB	II B	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	
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90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lw

- Group IV (elemental), III-V's, II-VI's, others...

Polymers

I A																	O	
1 H	II A											III A	IV A	V A	VIA	VII A	2 He	
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne	
11 Na	12 Mg	III B	IV B	V B	VII B	VIII					IB	II B	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	
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- Mainly organics, but not only...

What determines a material's performance?

Properties



Performance

Properties of Materials

- Mechanical
- Physical
 - Electrical
 - Thermal
 - Magnetic
 - Optical
 - Deteriorative
- Chemical
- Others

Properties



Performance

What determines a material's performance?

Structure



Properties



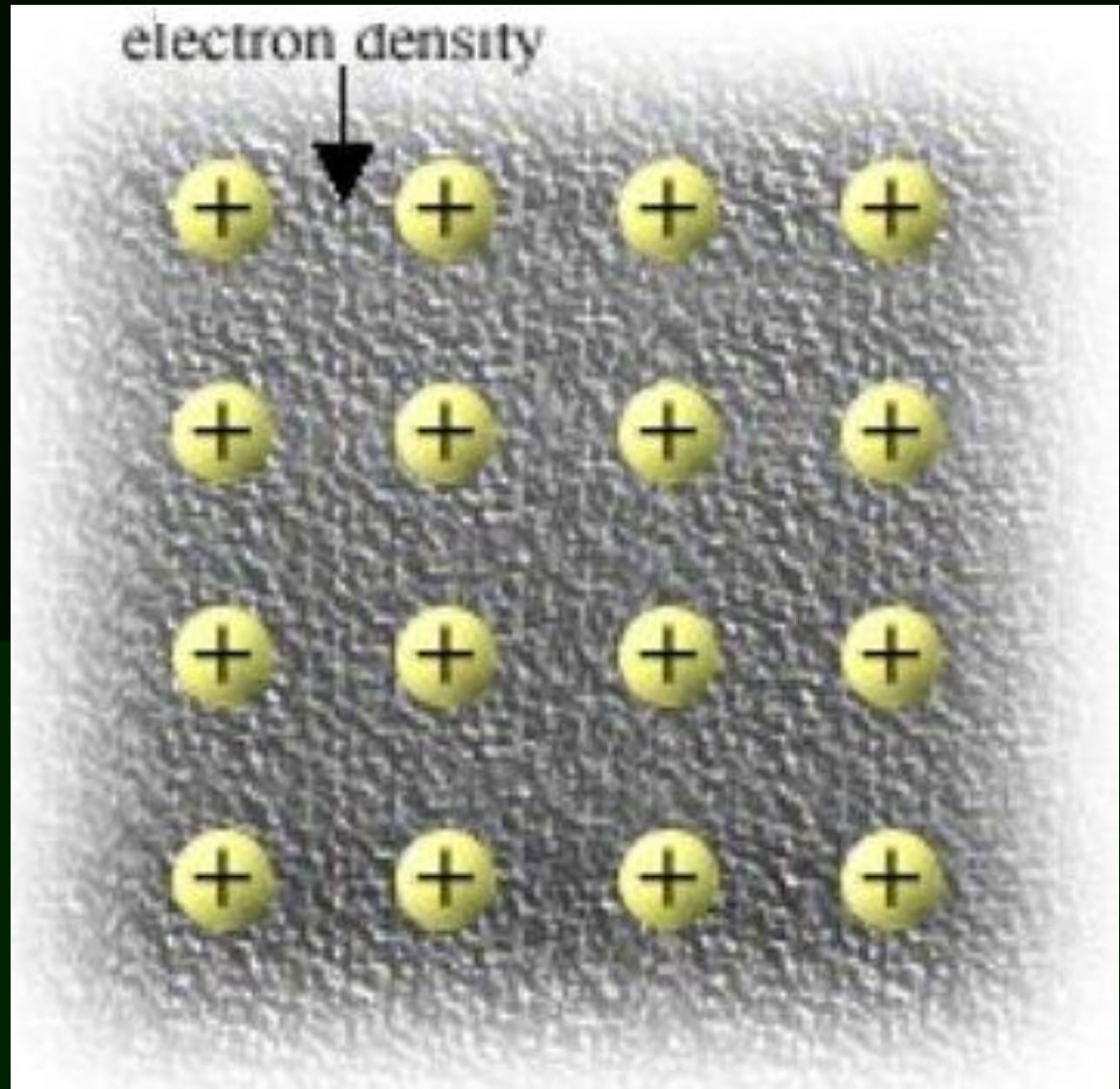
Performance

What do we mean by structure?

- Macroscopic
- Microscopic
- Mesoscopic
- Nanoscopic
- Atomic level

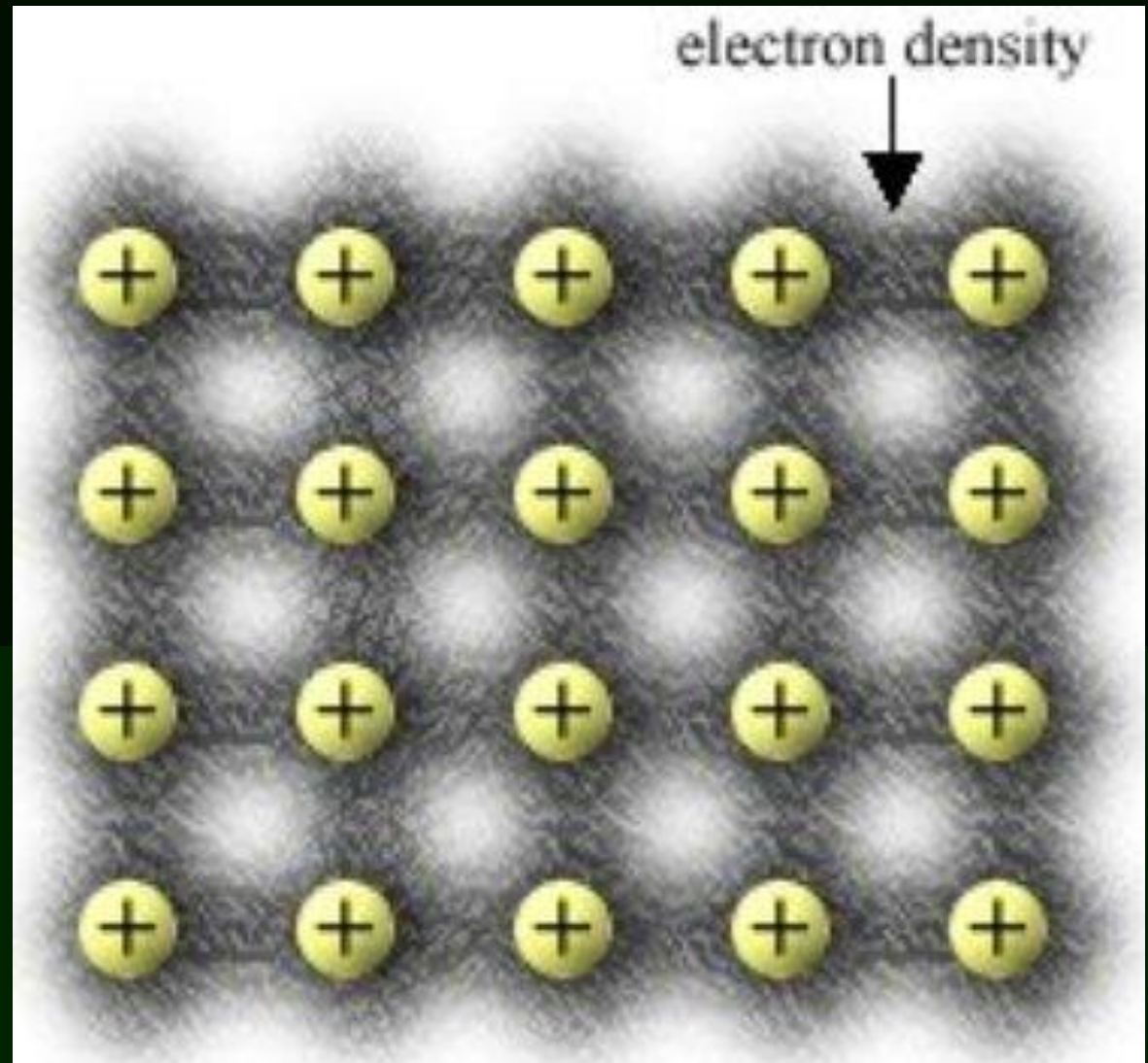
Bonding

- Metallic Bonding
 - Conductivity
 - Ductility
 - Heat capacity
 - Reactivity



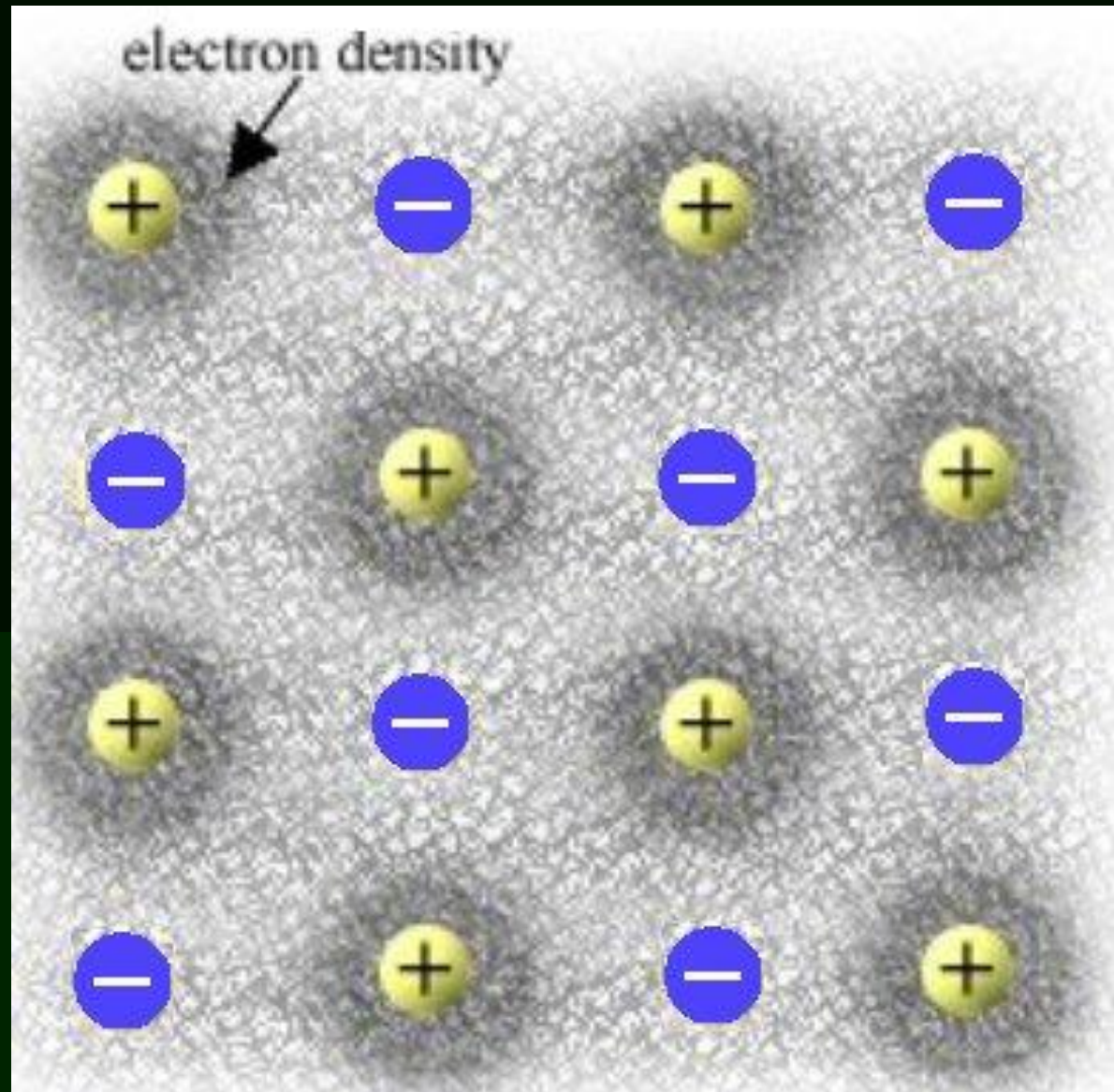
Bonding

- Covalent Bonding
 - Toughness
 - Brittleness
 - Insulation
 - Refractivity
 - Inactivity



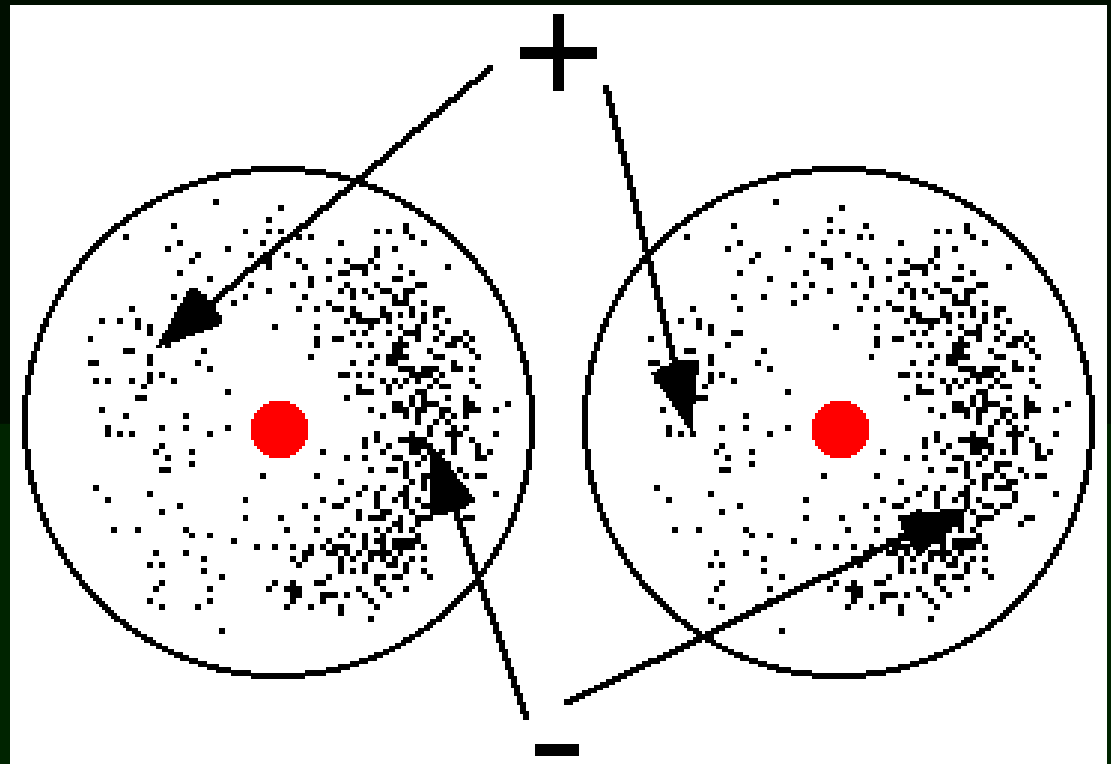
Bonding

- Ionic Bonding
 - Brittleness
 - Insulation
 - Reactivity



Bonding

- Van der Waals Bonding
 - Weakness
 - Insulation
 - Inactivity



Types of bonding in engineering materials

Material Type	Bonding Character	Example
Metal	Metallic	Iron, Cu
Ceramics and Glasses	Ionic/covalent	Silica (crystalline and amorphous)
Polymers	Covalent and secondary	Polyethylene
Semiconductors	Covalent or ionic/covalent	Si, CdS

Representation of Crystal Structures

- Atomic hard sphere model
- Packing density
- Lattices
- Unit cells
- Coordination spheres and polyhedra
- Point groups (of symmetry)
- Space groups
- 'Colour' groups

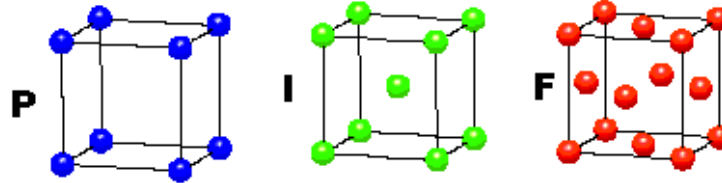
7 Crystal Systems

14 Crystal (Bravais) Lattices

CUBIC

$$a = b = c$$

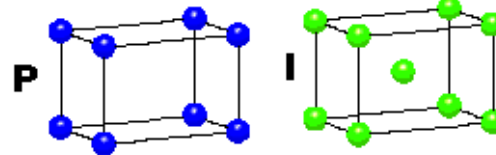
$$\alpha = \beta = \gamma = 90^\circ$$



TETRAGONAL

$$a = b \neq c$$

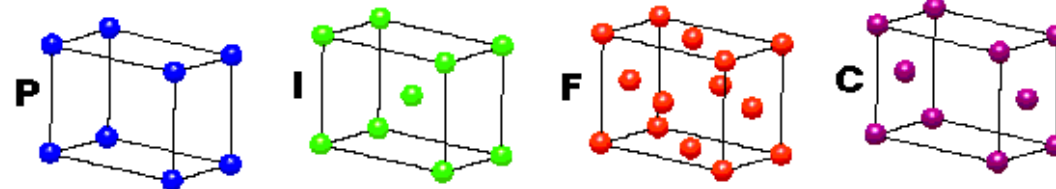
$$\alpha = \beta = \gamma = 90^\circ$$



ORTHORHOMBIC

$$a \neq b \neq c$$

$$\alpha = \beta = \gamma = 90^\circ$$

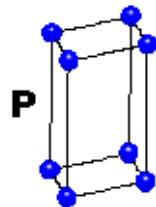


HEXAGONAL

$$a = b \neq c$$

$$\alpha = \beta = 90^\circ$$

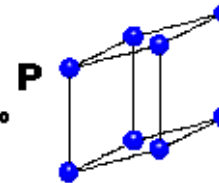
$$\gamma = 120^\circ$$



TRIGONAL

$$a = b = c$$

$$\alpha = \beta = \gamma \neq 90^\circ$$

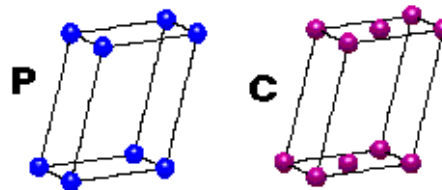


MONOCLINIC

$$a \neq b \neq c$$

$$\alpha = \gamma = 90^\circ$$

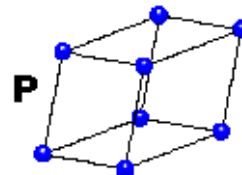
$$\beta \neq 120^\circ$$



TRICLINIC

$$a \neq b \neq c$$

$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$



4 Types of Unit Cell

P = Primitive

I = Body-Centred

F = Face-Centred

C = Side-Centred

+

7 Crystal Classes

→ 14 Bravais Lattices

Atomic Packing Factor

$$APF = \frac{\text{Volume of atoms in a unit cell}}{\text{Total volume of unit cell}}$$

Homework

Calculate the APF for

- (Primitive) cubic
 - BCC
 - FCC

Crytallographic Points, Directions and Planes

- Set up right-handed set of axes x , y , and z
 - x , y , and z along the edges of a unit cell
 - Origin at a lattice point
 - x , y , and z not always mutually perpendicular!
 - a , b , and c are the unit length of the three corresponding unit cell edges
- Labelling conventions

	<u>Points</u>	<u>Directions</u>	<u>Planes</u>
	101	[110]	(110)
	$\bar{1}\bar{1}1$	$[\bar{1}\bar{1}1]$	(100)
Families		{001}	<011>

What determines a material's performance?

Process → Structure → Properties → Performance

Basic aim of this short course

- Understand how processing affects the
 - Structure
 - Properties
 - Performanceof materials
- Concentrate (focus and emphasis) on metals, semiconductors, oxides...