

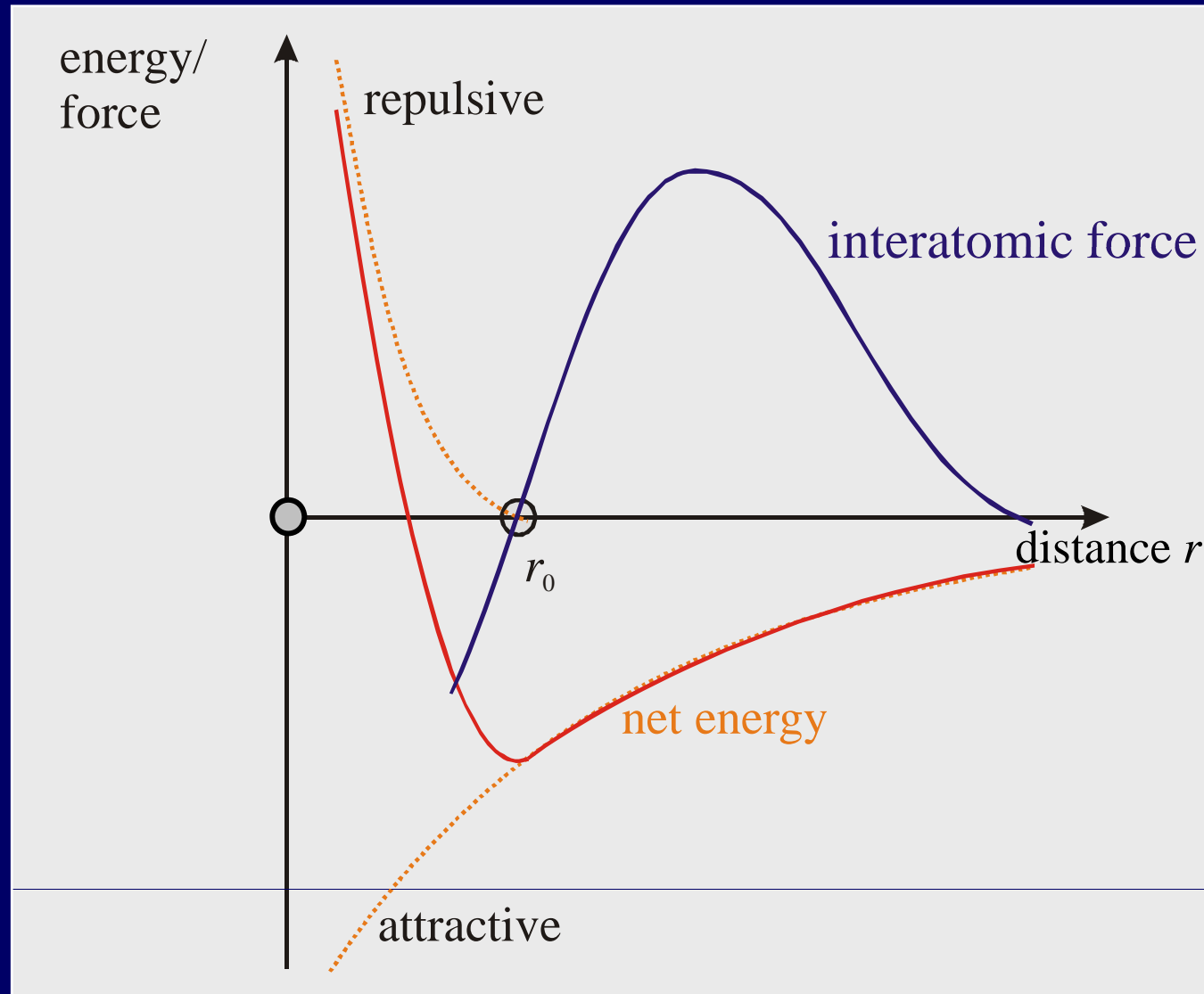
last lecture

- Introduction to materials science and engineering
- Atoms / electron configuration

today

- Bonding in solids
- Structure of crystal solids

Bonding Forces and Energies



The Periodic Table

IA																												0				
1																		2														
H																		He														
2.1																		-														
3	4											5	6	7	8	9																
Li	Be											B	C	N	O	F																
1.0	1.5											2.0	2.5	3.0	3.5	4.0																
11	12											13	14	15	16	17	18															
Na	Mg											Al	Si	P	S	Cl	Ar															
0.9	1.2											1.5	1.8	2.1	2.5	3.0	-															
		IIIB	IVB	VB	VIB	VII B	VIII			IB	IIB																					
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															
0.8	1.0	1.3	1.5	1.6	1.6	1.5	1.8	1.8	1.8	1.9	1.6	1.6	1.8	2.0	2.4	2.8	-															
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															
0.8	1.0	1.2	1.4	1.6	1.8	1.9	2.2	2.2	2.2	1.9	1.7	1.7	1.8	1.9	2.1	2.5	-															
55	56	57-71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86															
Cs	Ba	La-Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn															
0.7	0.9	1.1-1.2	1.3	1.5	1.7	1.9	2.2	2.2	2.2	2.4	1.9	1.8	1.8	1.9	2.0	2.2	-															
87	88	89-102																														
Fr	Ra	Ac-No																														
0.7	0.9	1.1-1.7																														

increasing electronegativity

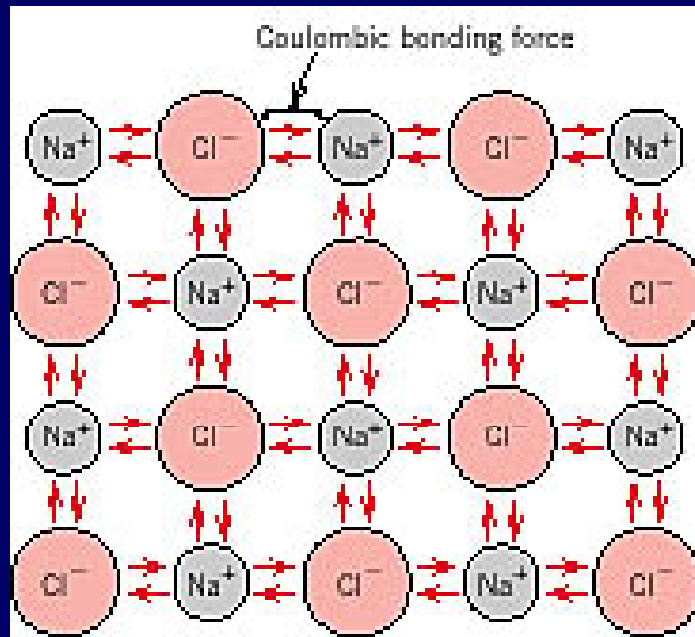
METALS

INTERMEDIATE

NONMETALS

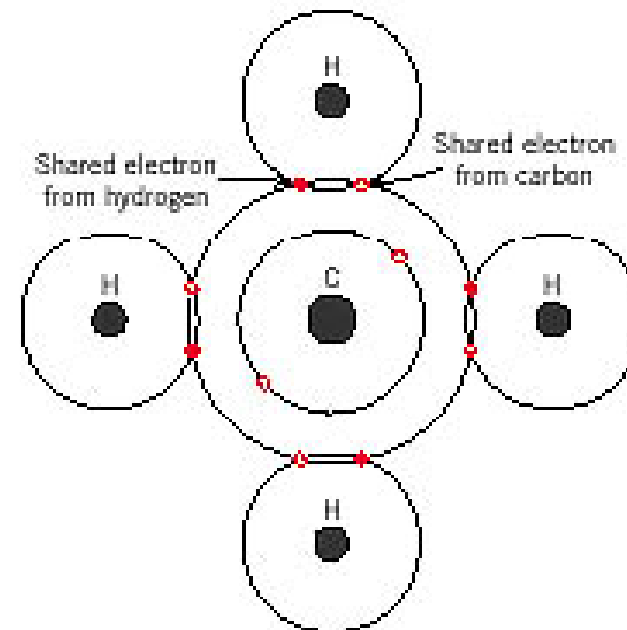
Ionic Bonding

e.g. sodium chloride

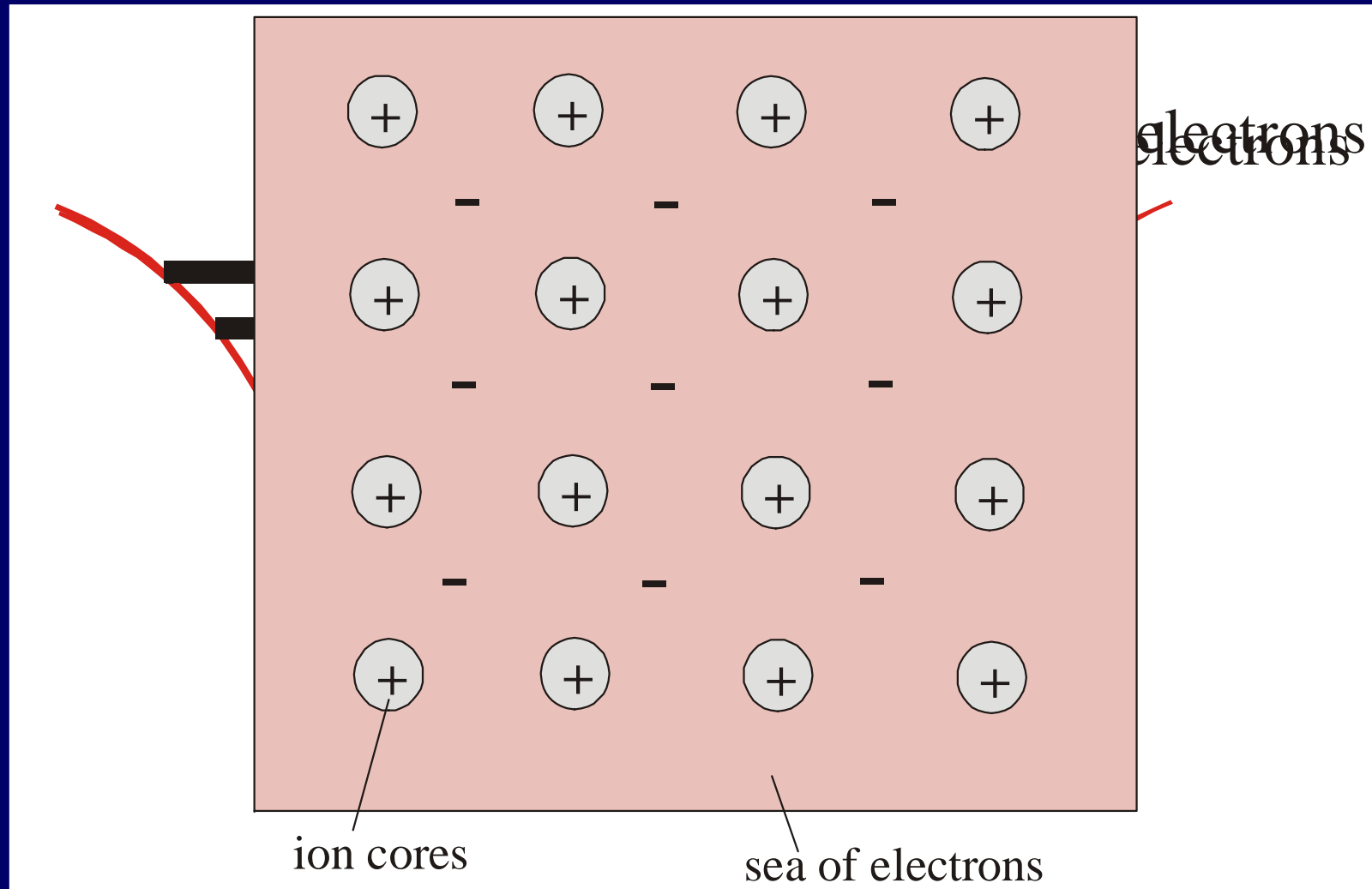


Covalent Bonding

e.g. methane



Metallic Bonding



Bonding Energies

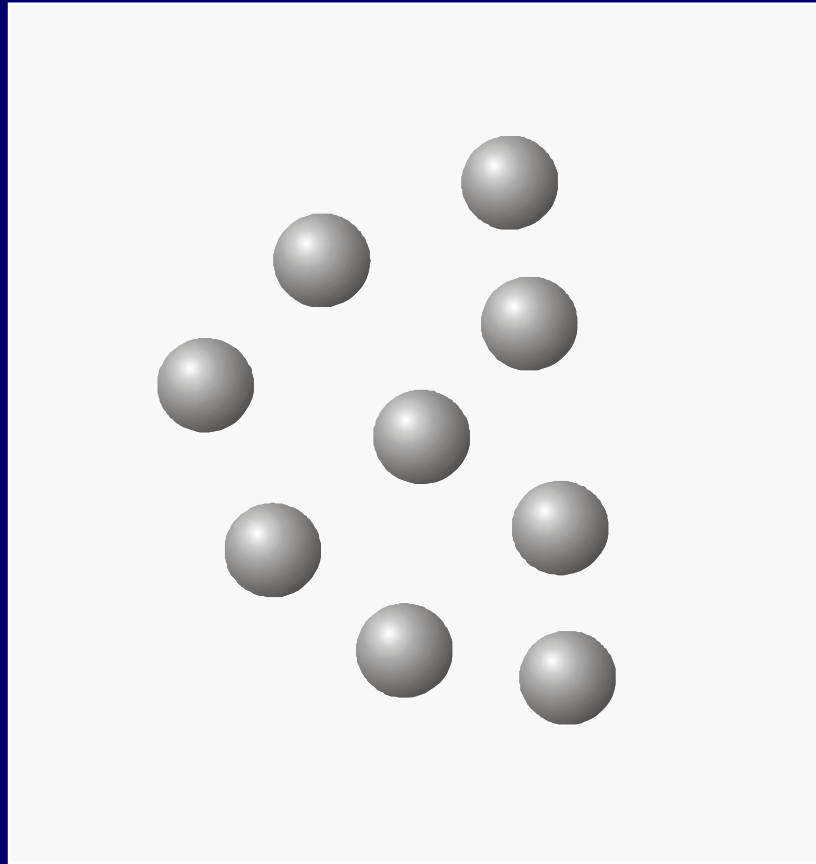
<i>Bonding Type</i>	<i>Substance</i>	<i>Bonding Energy</i>		<i>Melting Temperature (°C)</i>
		<i>kJ/mol (kcal/mol)</i>	<i>eV/Atom, Ion, Molecule</i>	
Ionic	NaCl	640 (153)	3.3	801
	MgO	1000 (239)	5.2	2800
Covalent	Si	450 (108)	4.7	1410
	C (diamond)	713 (170)	7.4	>3550
Metallic	Hg	68 (16)	0.7	-39
	Al	324 (77)	3.4	660
	Fe	406 (97)	4.2	1538
	W	849 (203)	8.8	3410

high

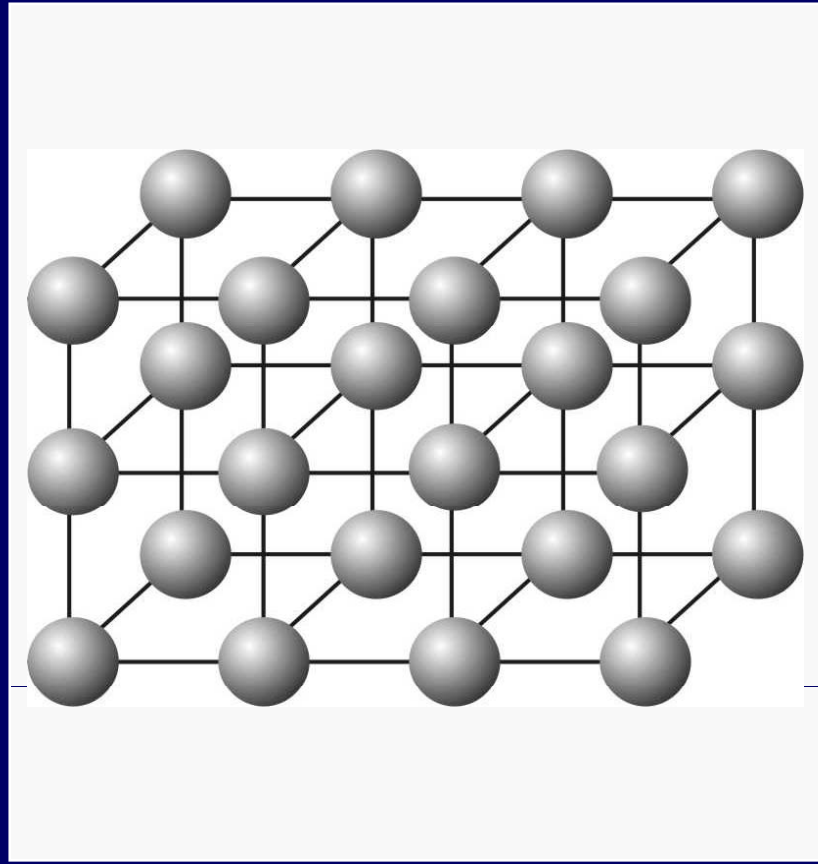
Crystalline Structures

Crystalline Structures

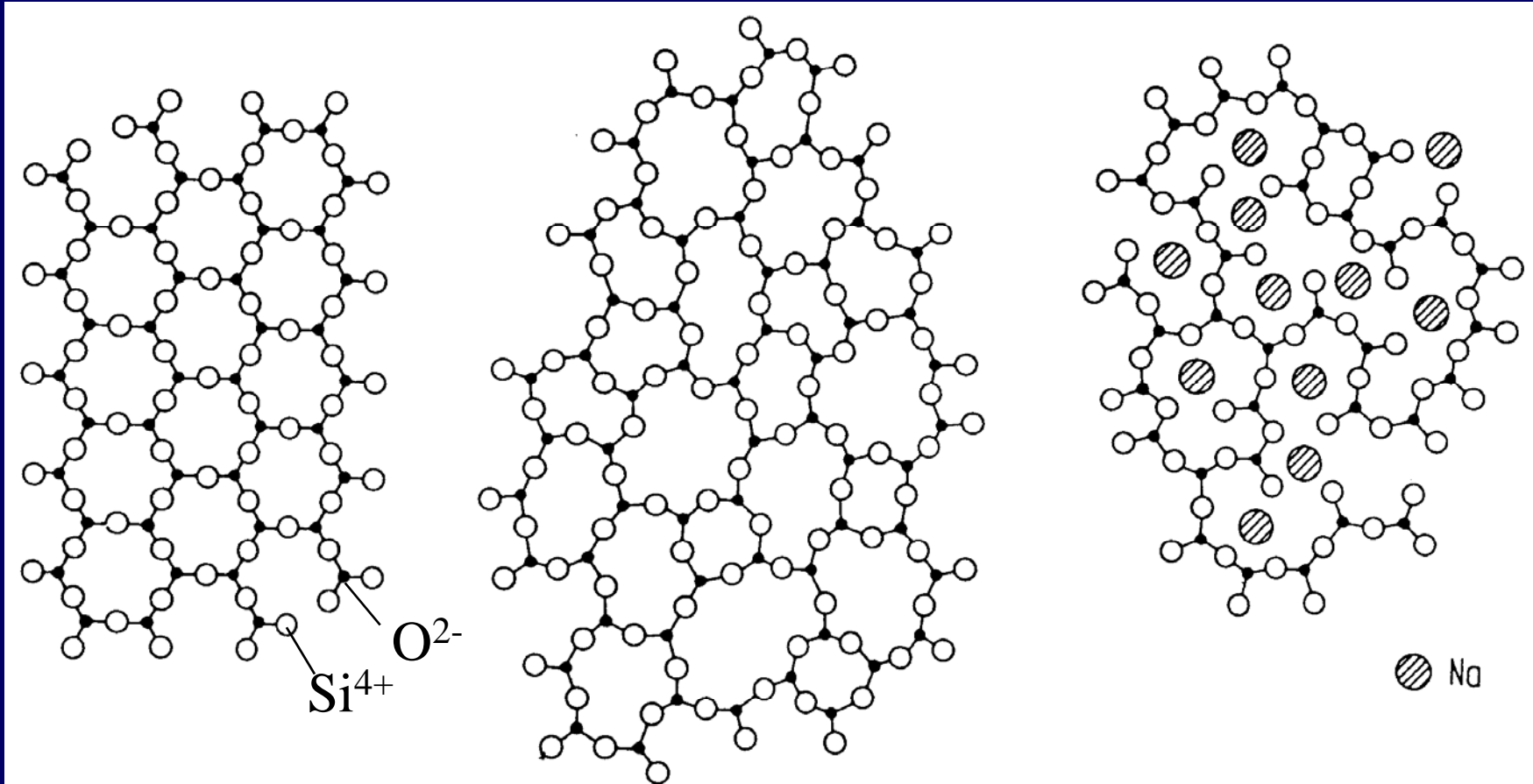
amorphous



crystalline



Example: Glass

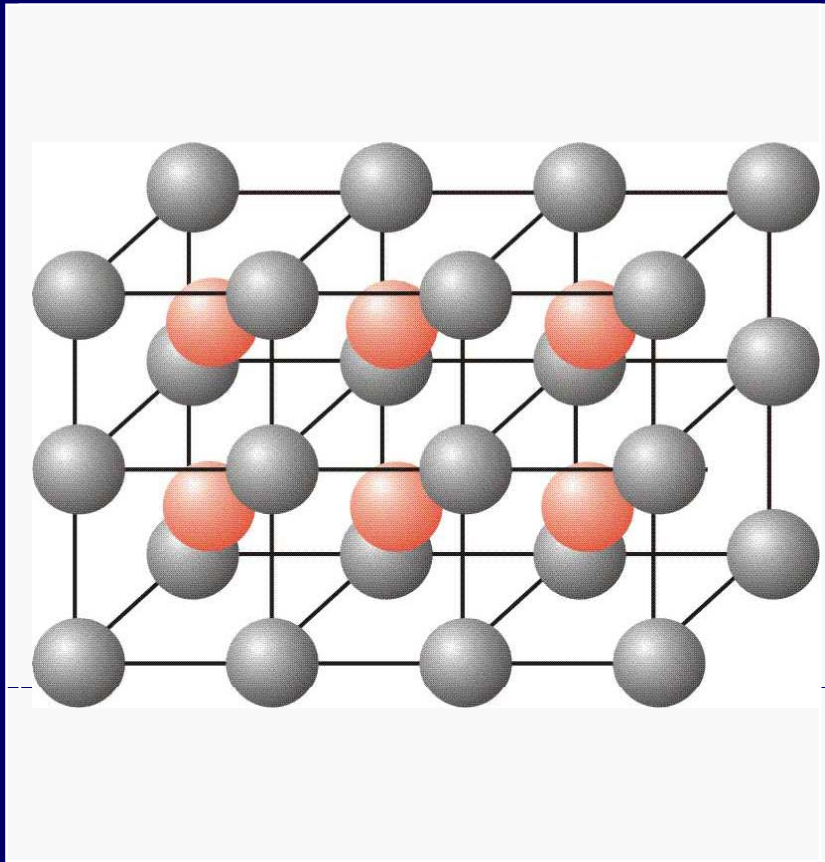


quartz
(crystalline)

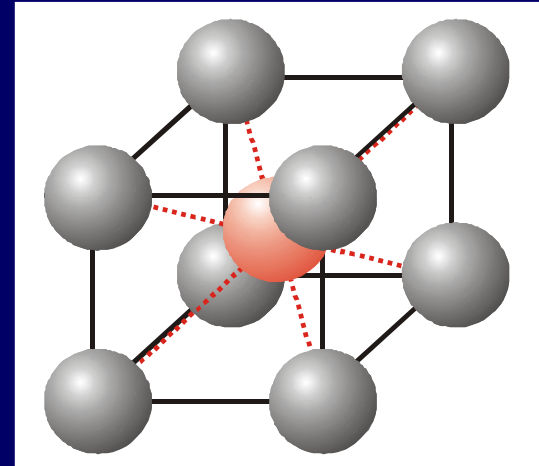
quartz glass
(amorphous)

glass
(amorphous)

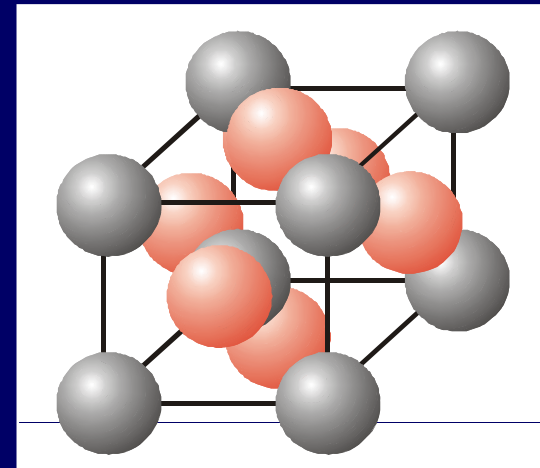
Crystalline Structures



body-centered cubic (bcc)



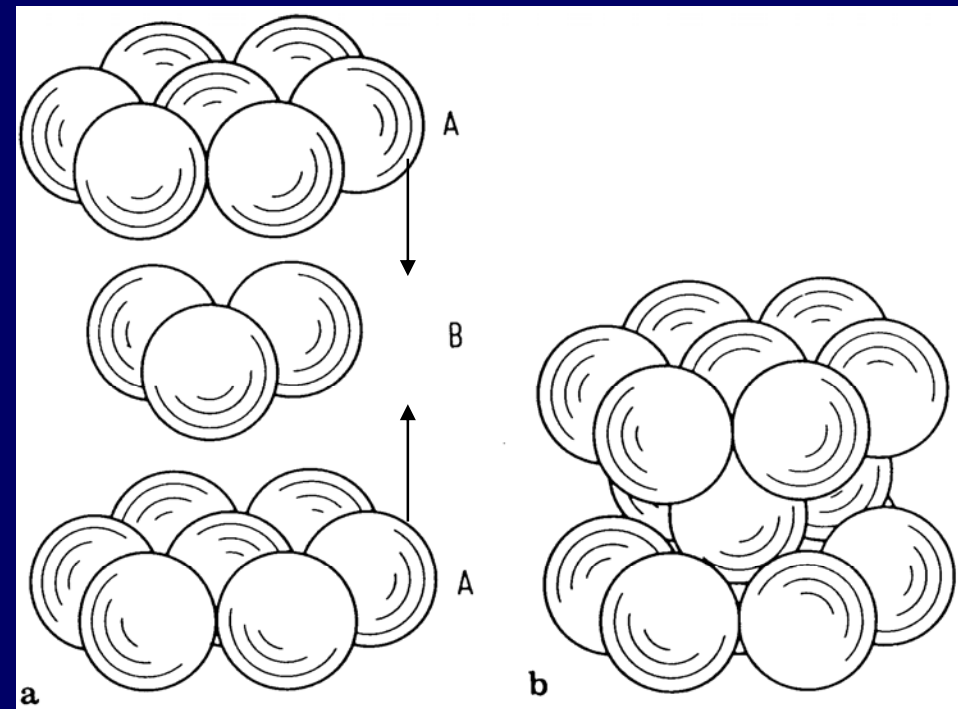
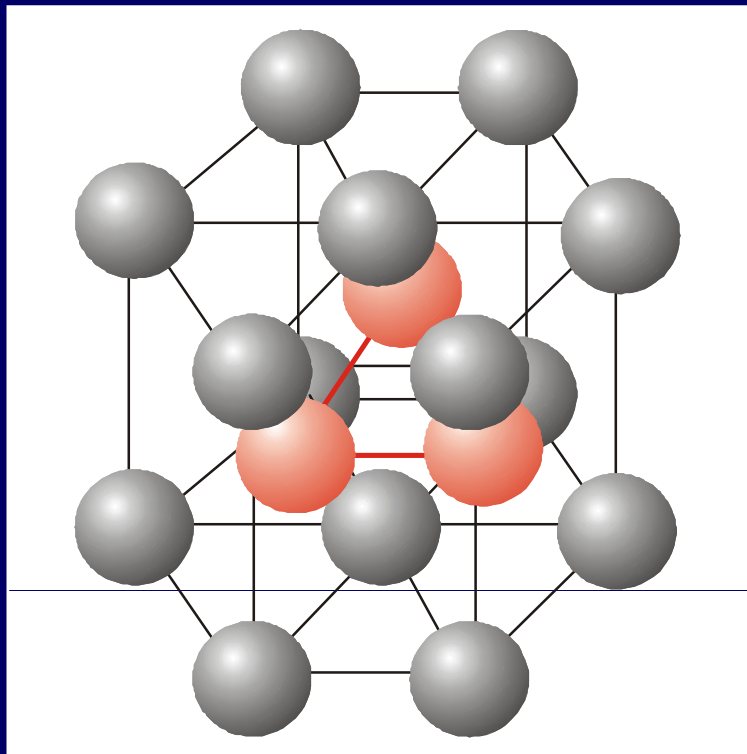
bcc



fcc

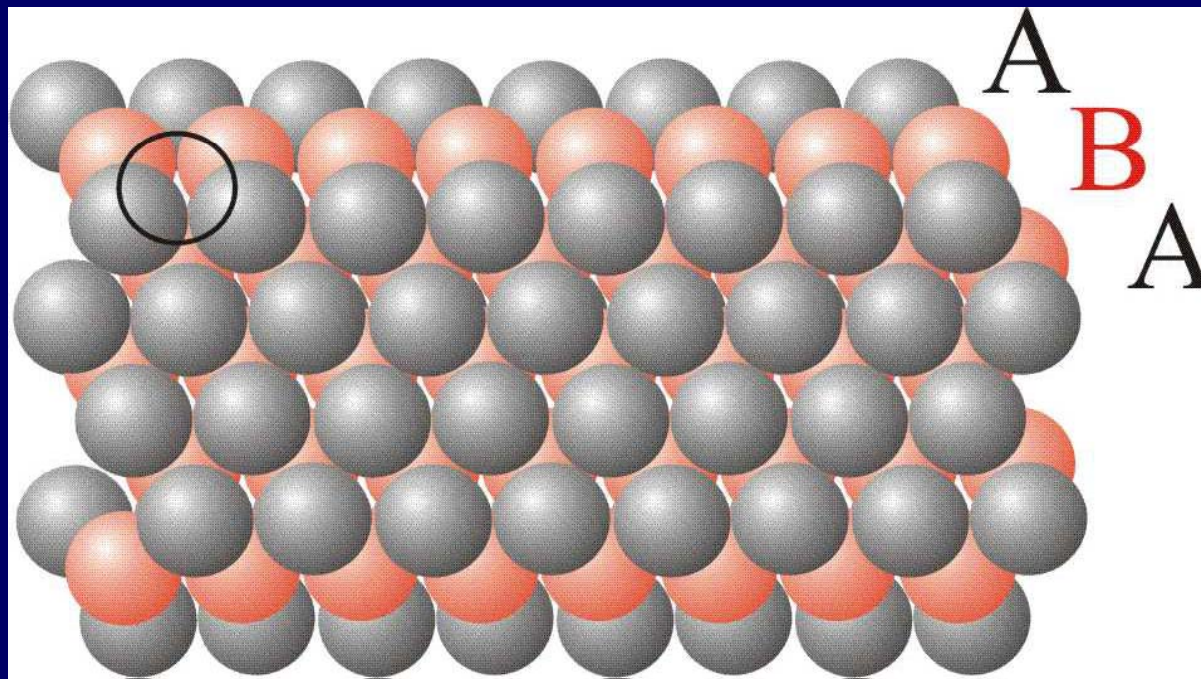
Hexagonal Crystal Structures

hcp unit cell



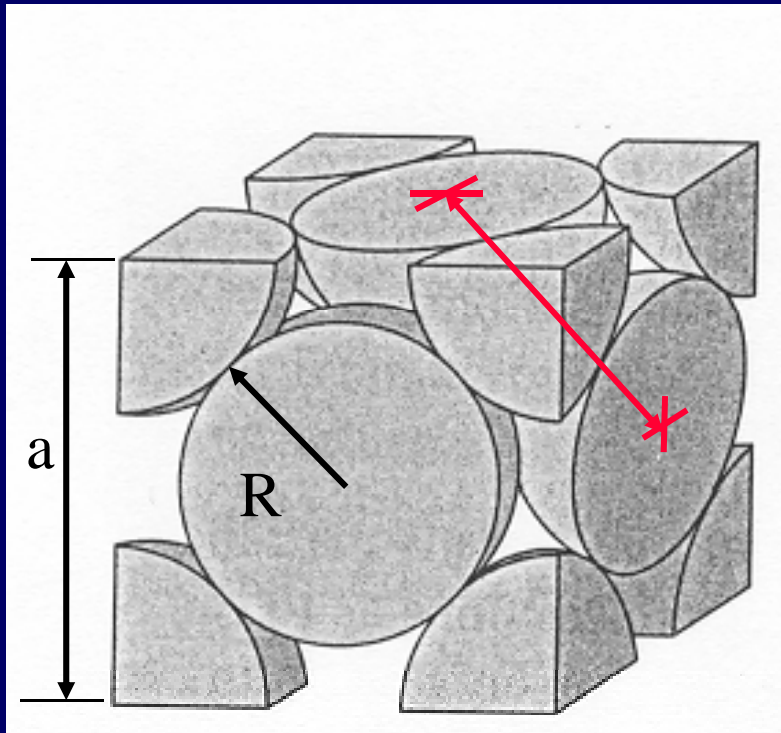
Stacking Sequence of Close-Packed Structures

first plane A, second plane B and third plane A: fcc

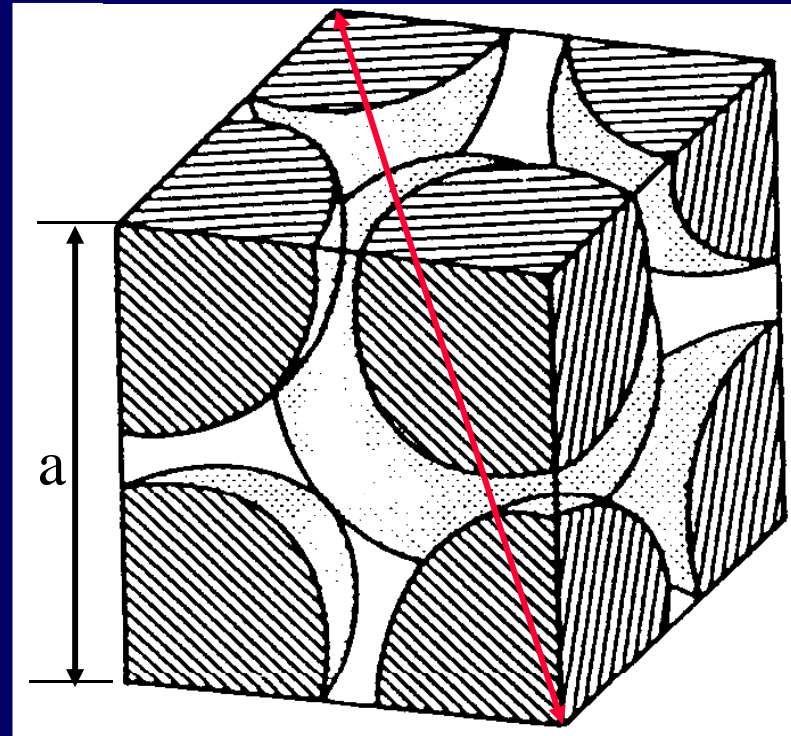


FCC and BCC Solid Sphere Model

fcc unit cell



bcc unit cell



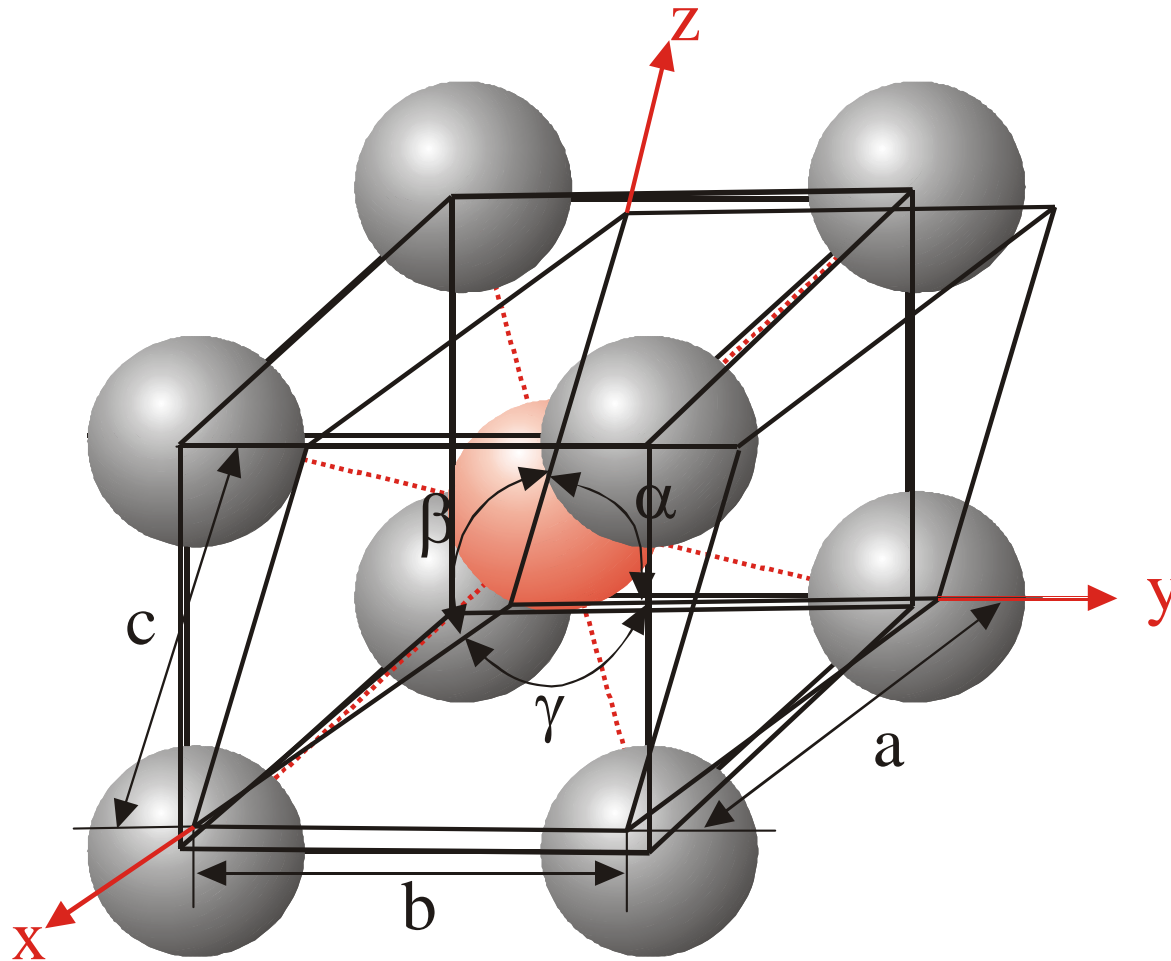
R = atomic radius

a = unit cell length / lattice constant

Crystalline Structures of Materials

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											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															
Lanthanoide			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	
Aktinoide			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		

Lattice Parameters

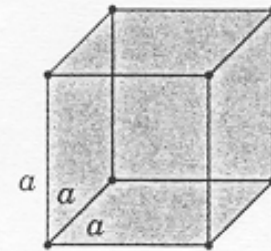


Crystal Systems

Cubic

$$a = b = c$$

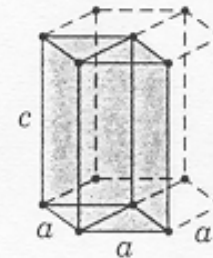
$$\alpha = \beta = \gamma = 90^\circ$$



Hexagonal

$$a = b \neq c$$

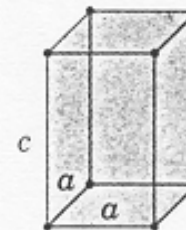
$$\alpha = \beta = 90^\circ, \gamma = 120^\circ$$



Tetragonal

$$a = b \neq c$$

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

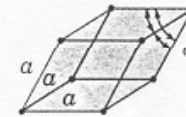


Crystal Systems

Rhombohedral

$$a = b = c$$

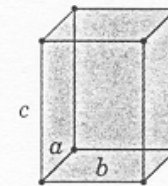
$$\alpha = \beta = \gamma \neq 90^\circ$$



Orthorhombic

$$a \neq b \neq c$$

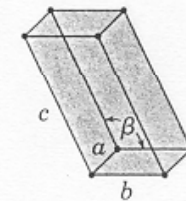
$$\alpha = \beta = \gamma = 90^\circ$$



Monoclinic

$$a \neq b \neq c$$

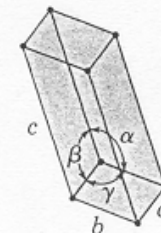
$$\alpha = \gamma = 90^\circ \neq \beta$$



Triclinic

$$a \neq b \neq c$$

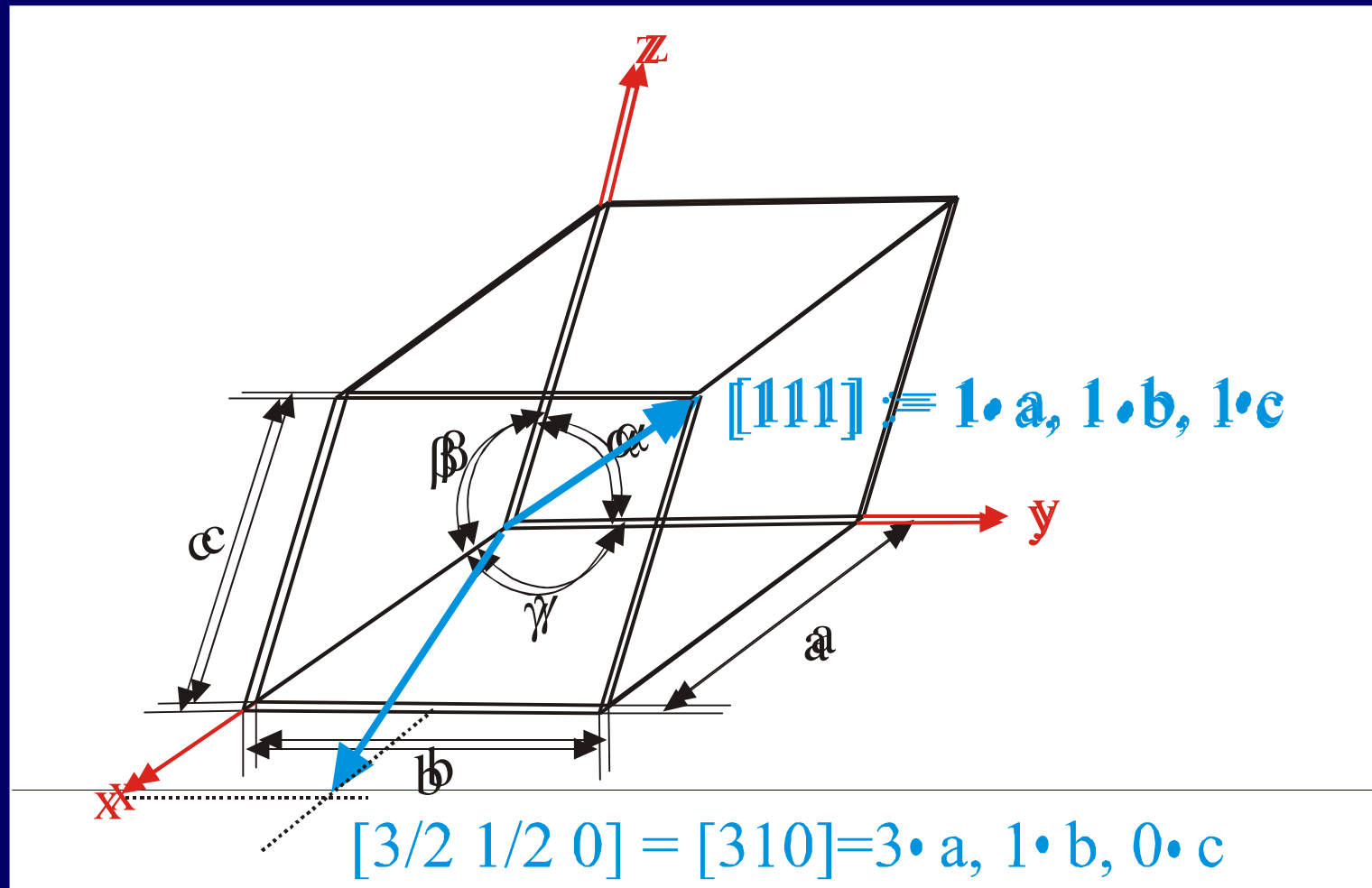
$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$



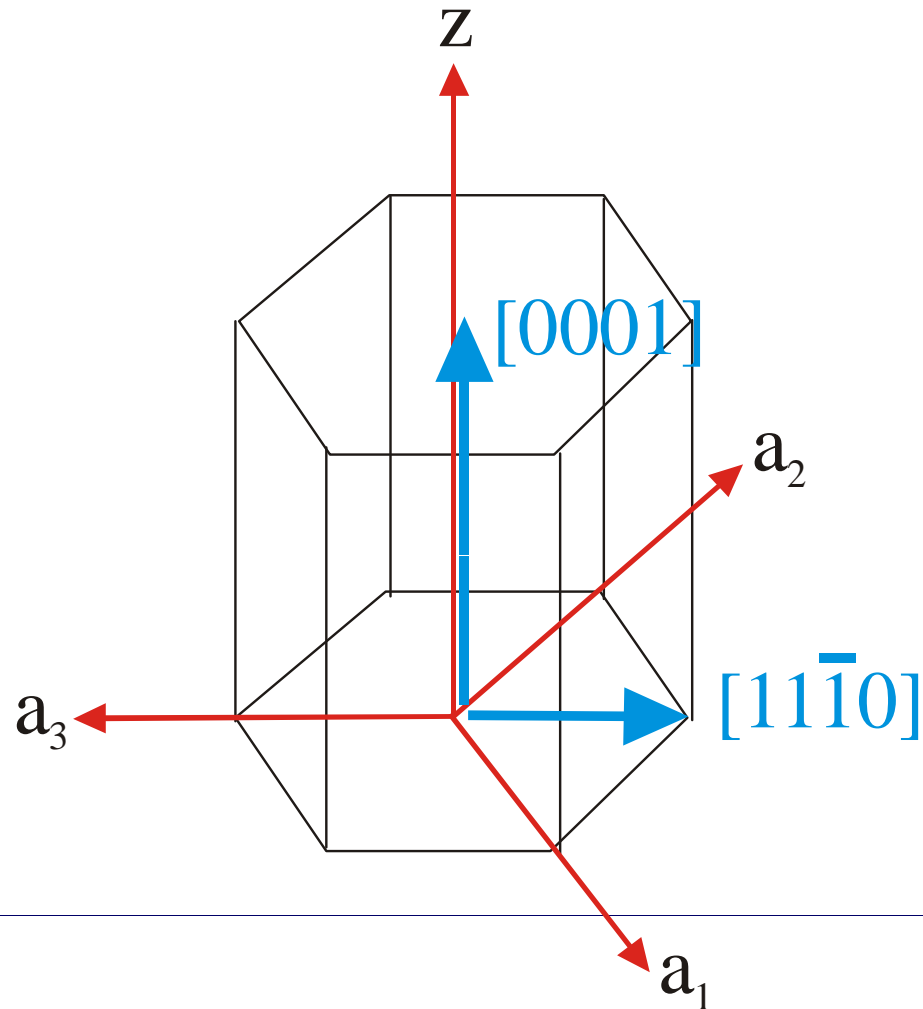
How to define a direction

- Vector of convenient length (pass through origin)
- Project the vector to the axes (and measure in a, b, and c)
- Multiply or divide these numbers by common factor to get smallest set of integers
- Write them down as [uvw]

Miller Indices: Crystallographic Directions



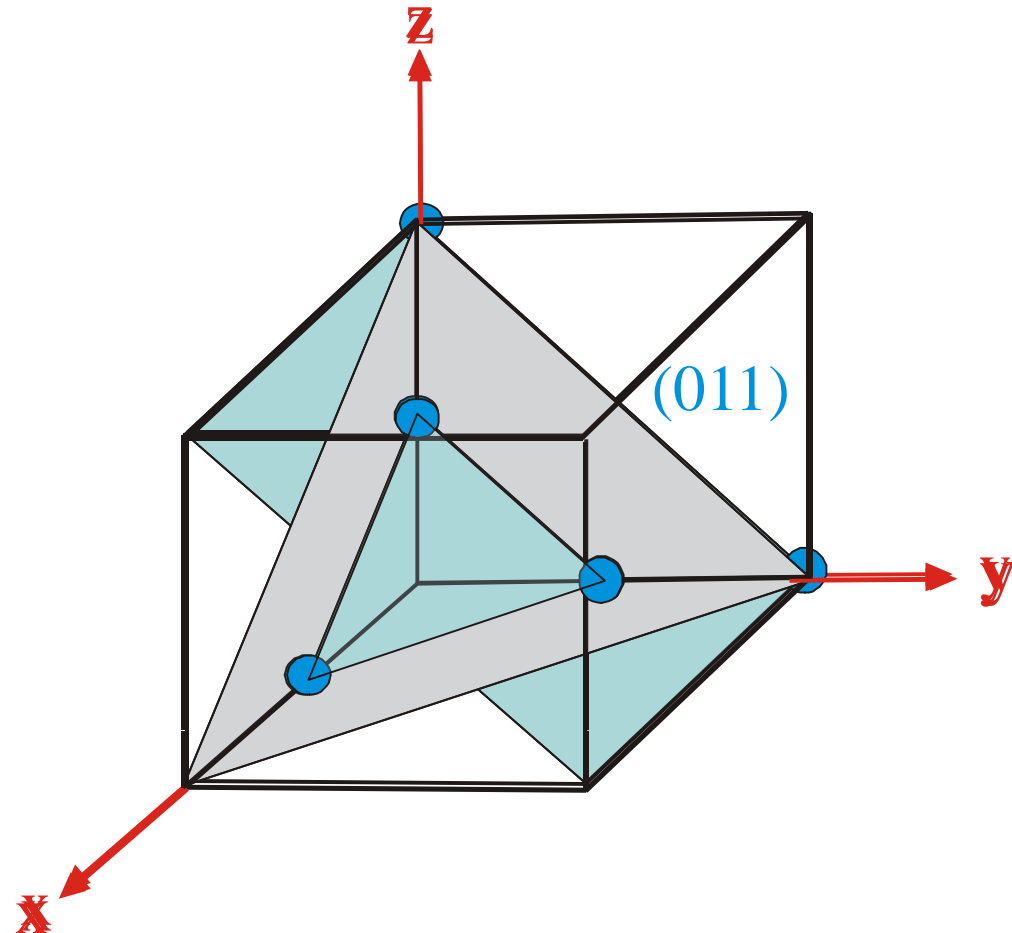
Miller Indices: Crystallographic Directions (Miller Bravais)



How to define a plane

- Plane may not include origin!
- Determine the intercepts with appropriate axes as a , b , and c
- Take reciprocals (no intercept means infinity \rightarrow reciprocal of infinity = 0)
- Multiply or divide these numbers by common factor to get smallest set of integers
- Write them down as (hkl)

Miller Indices: Lattice Planes

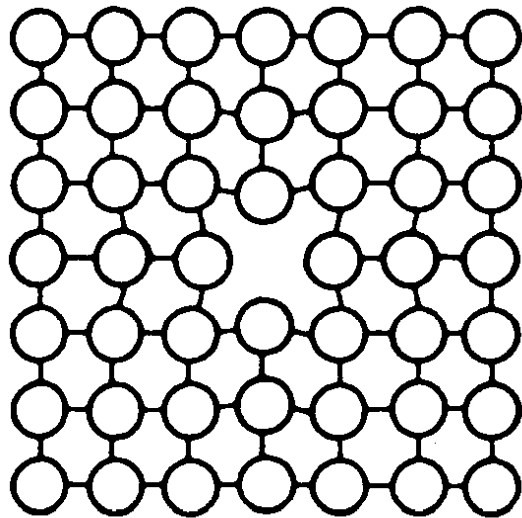


Defects

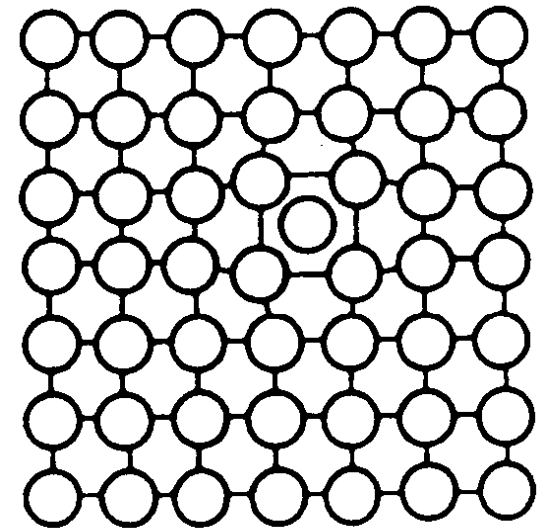
- Point defects
- Linear defects
- 2-dimensional defects

Point Defects

vacancy

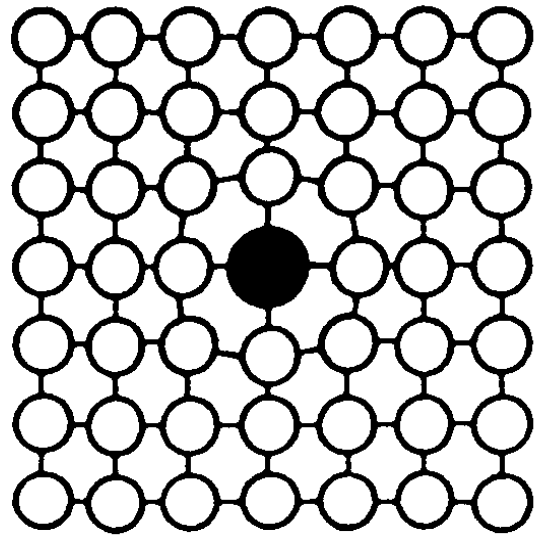


self-interstitial

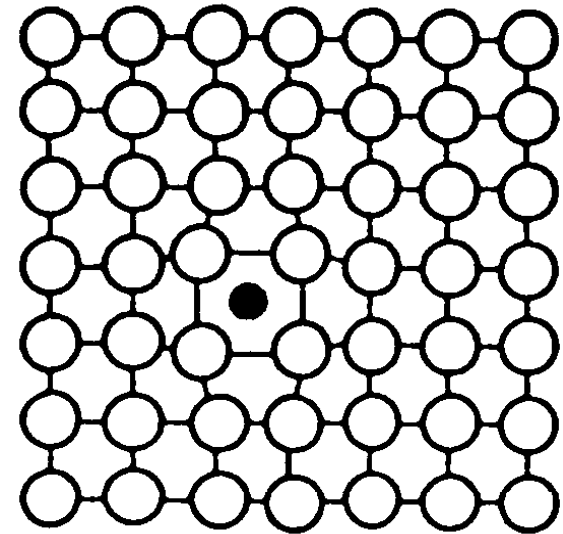


Impurity Atoms

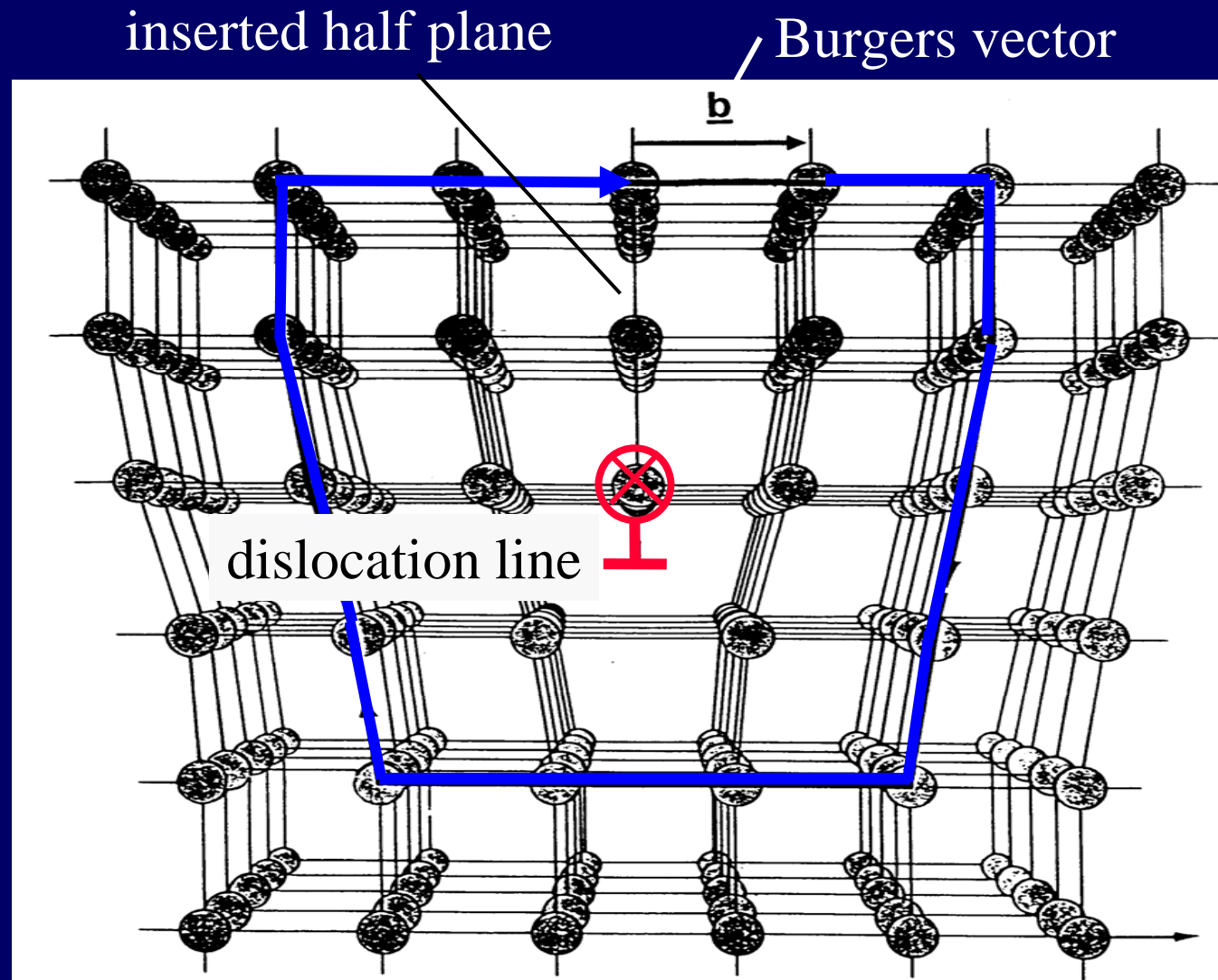
substitutional



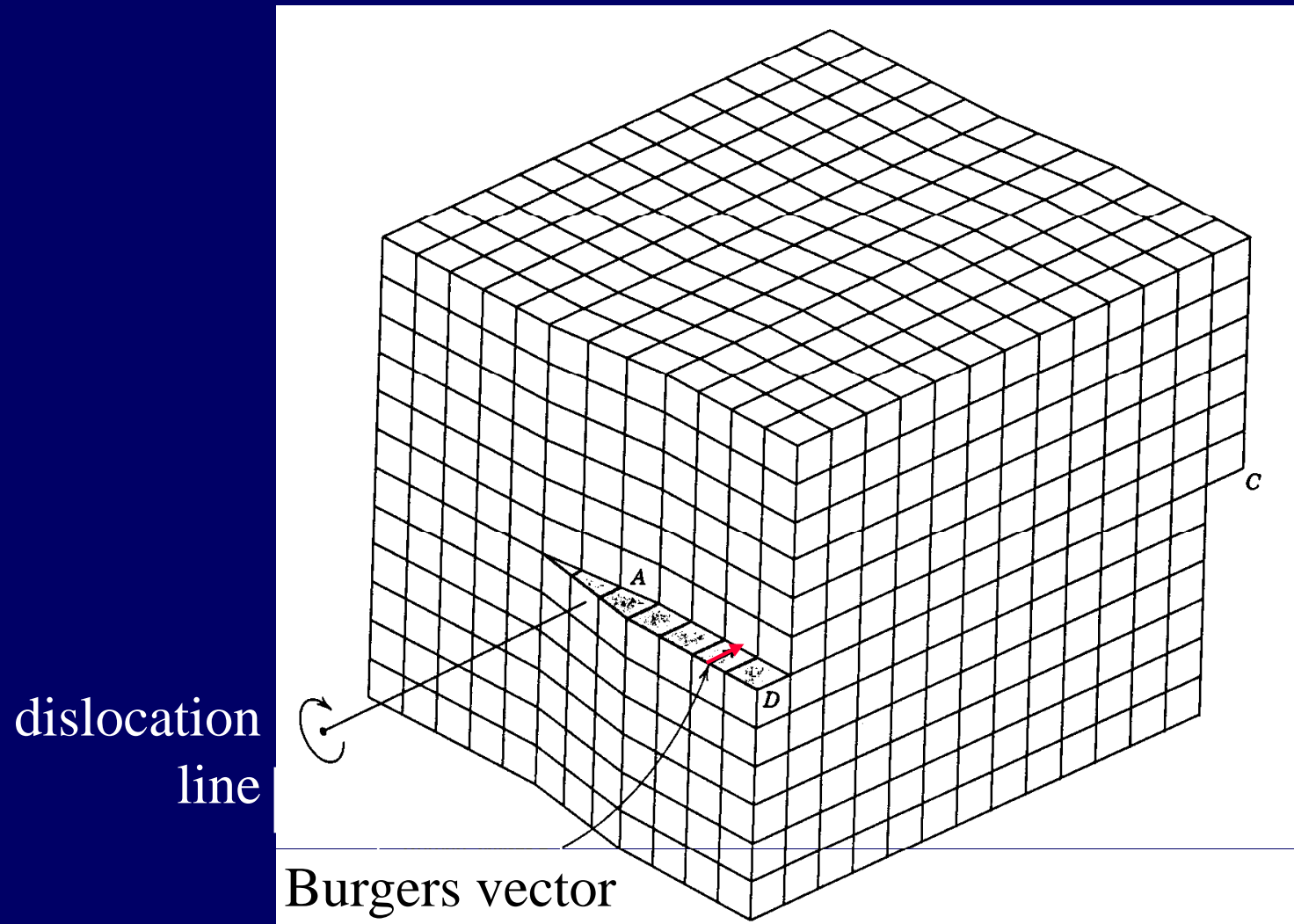
interstitial



Dislocations: Edge Dislocation

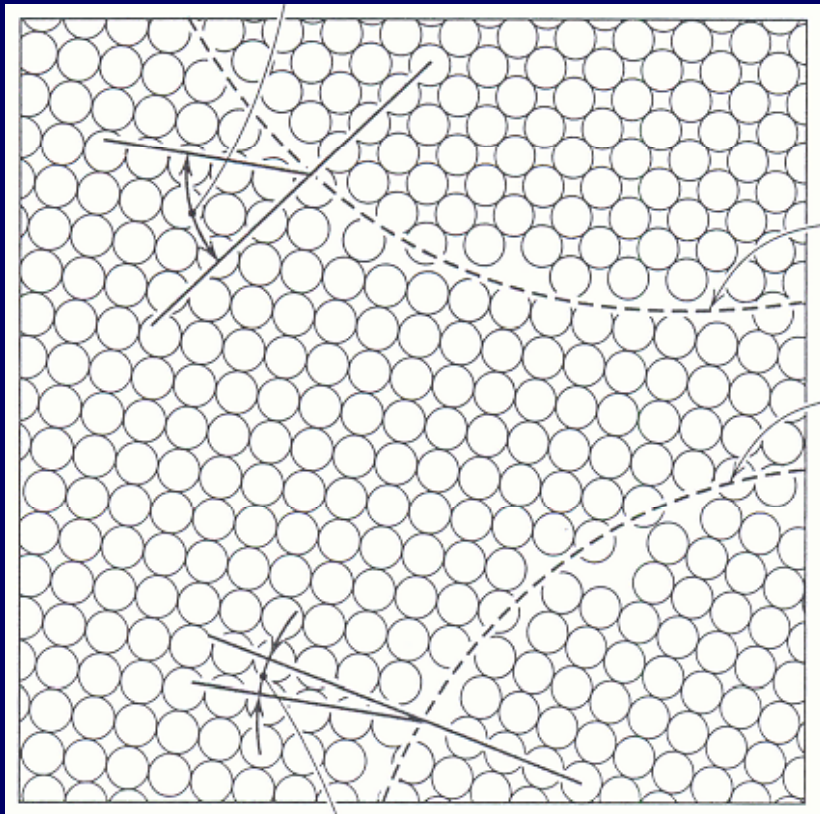


Dislocations: Screw Dislocation



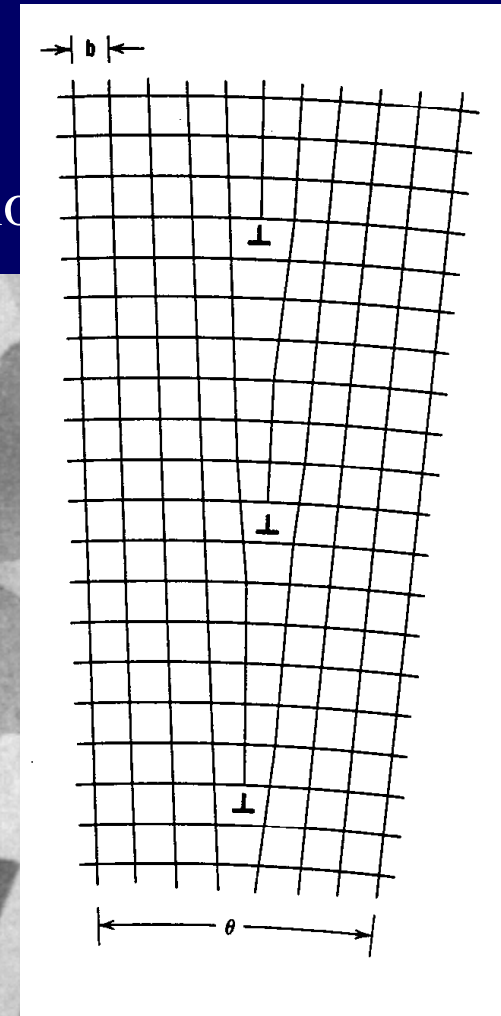
Grain Boundaries

high-angle grain boundary ($\Theta > 15^\circ$)



Ni-Base Superalloy

low-angle
grain boundary



50μm

next

- Properties of materials