

Homework for Chapter 1

#1.1 + #1.2

Homework #1.1 for Chapter 1 (A1, 3, 5, 10, 13, 15,)

A1. In a unit cell, **an atom's coordination number** is the number of atoms it is touching (the closest vicinity of the atom). (配位數是晶格中與某一原子相距最近的原子個數.) What are the coordination number for sc, bcc, fcc, hcp, and diamond lattices?

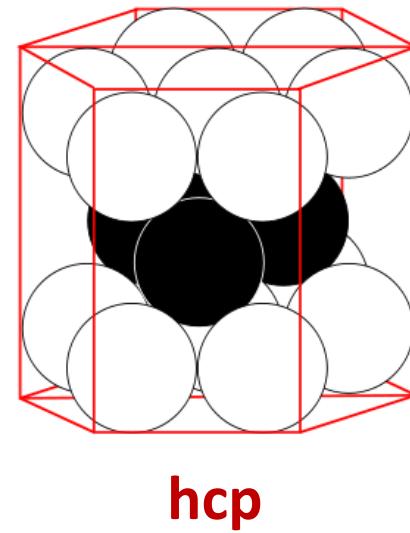
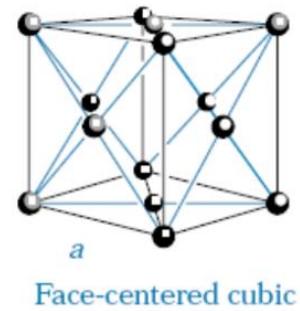
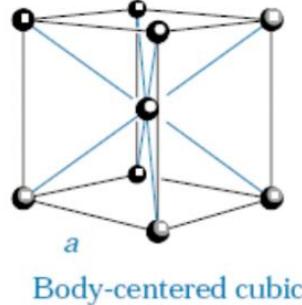
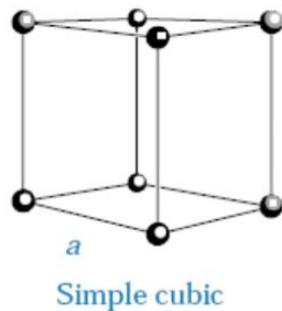


Figure 1-3

Unit cells for three types of cubic lattice structures.

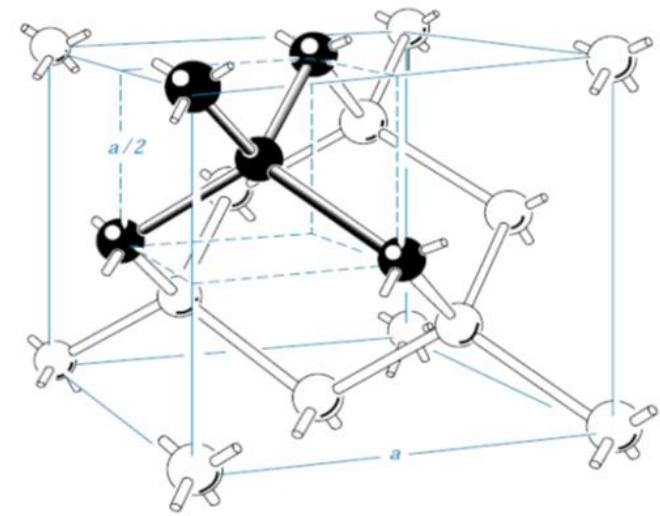
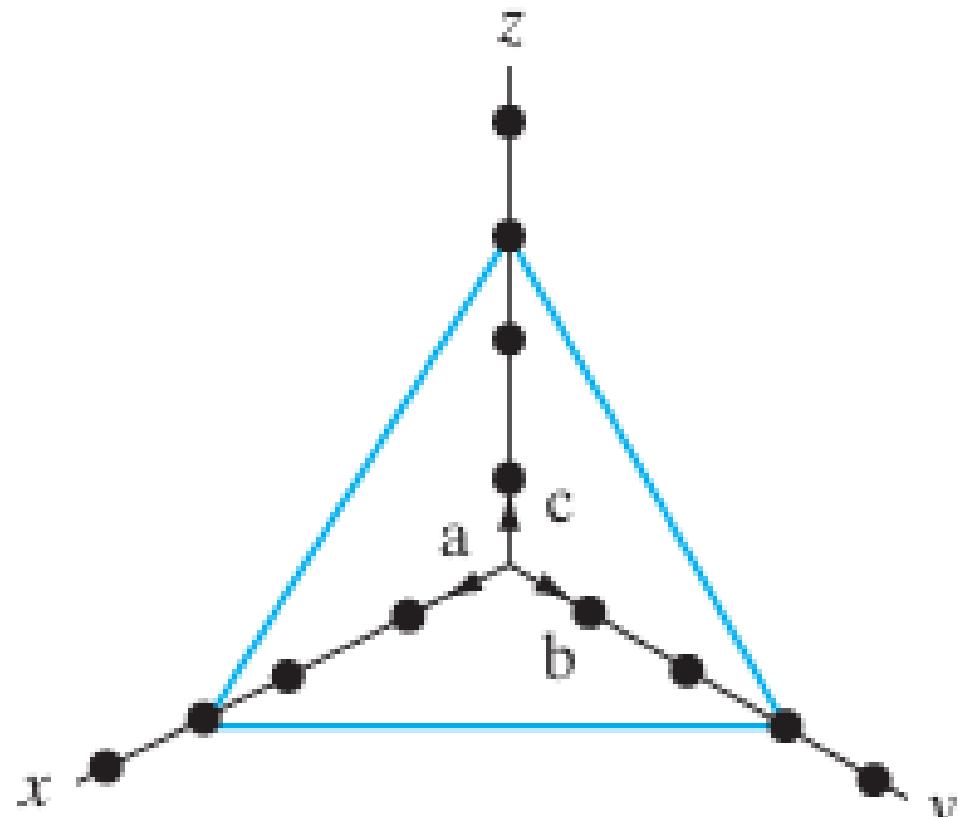


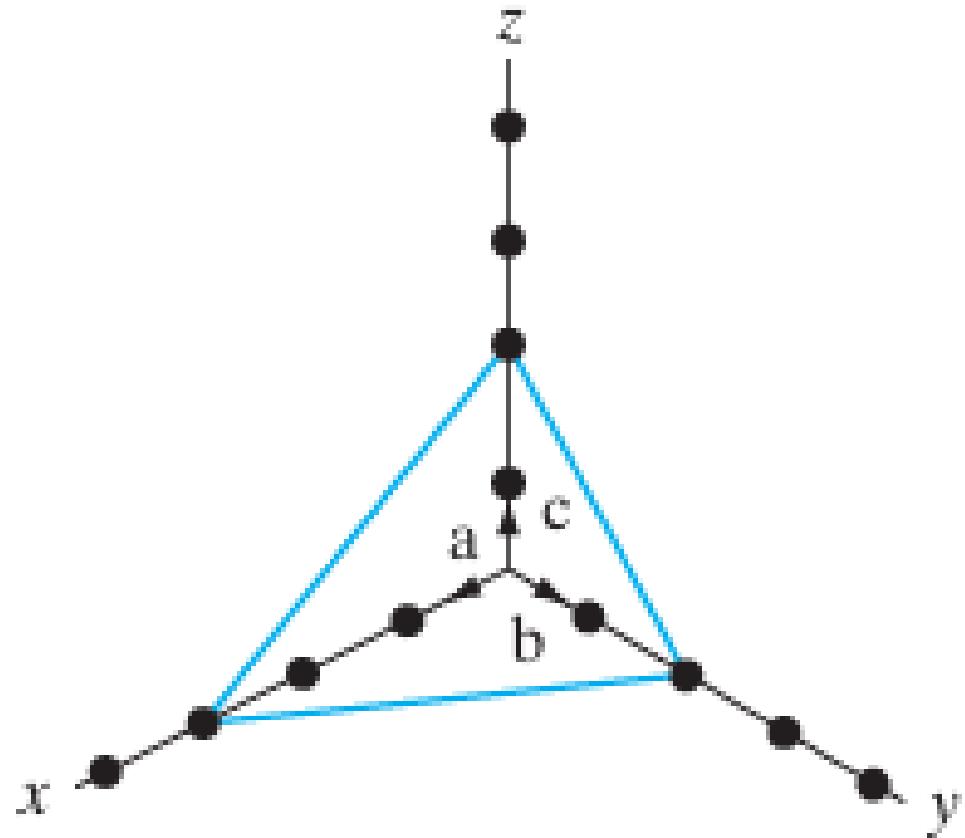
Figure 1-9

1.3 Label the planes illustrated in Fig. P1-3.

In terms of Miller indices (密勒指數) (hkl)



(a)



(b)

1.5 Calculate the densities of Si and GaAs from the lattice constants (Appendix III), atomic weights, and Avogadro's number. Compare the results with densities given in Appendix III. The atomic weights of Si, Ga, and As are 28.1, 69.7, and 74.9, respectively.

1.10 (a) Find the number of atoms/cm² on the (100) surface of a Si wafer.
(b) What is the distance (in Å) between nearest In neighbors in InP.

1.13 How many atoms are found inside a unit cell of an sc, a bcc, and an fcc crystal? How far apart in terms of lattice constant a are the nearest neighbor atoms in each case, measured from center to center?

1.15 Find the maximum fractions of the unit cell volume that can be filled by hard spheres in the sc, fcc, and diamond lattices.



Appendix III

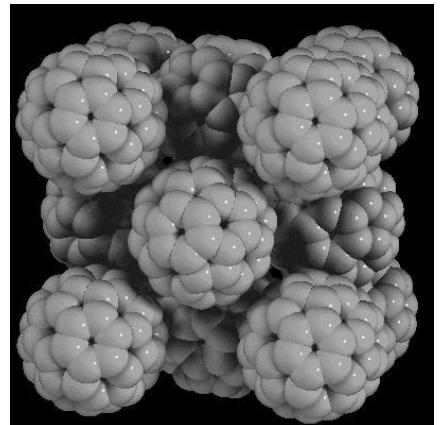
		E_g (eV)	μ_n (cm ² /V-s)	μ_p (cm ² /V-s)	m_n^*/m_o (m_l/m_i)	m_p^*/m_o (m_{lh}/m_{hh})	a (Å)	ϵ_r	Density (g/cm ³)	Melting point (°C)
Si	(i/D)	1.11	1350	480	0.98, 0.19	0.16, 0.49	5.43	11.8	2.33	1415
Ge	(i/D)	0.67	3900	1900	1.64, 0.082	0.04, 0.28	5.65	16	5.32	936
SiC (α)	(i/W)	2.86	500	—	0.6	1.0	3.08	10.2	3.21	2830
AlP	(i/Z)	2.45	80	—	—	0.2, 0.63	5.46	9.8	2.40	2000
AlAs	(i/Z)	2.16	1200	420	2.0	0.15, 0.76	5.66	10.9	3.60	1740
AlSb	(i/Z)	1.6	200	300	0.12	0.98	6.14	11	4.26	1080
GaP	(i/Z)	2.26	300	150	1.12, 0.22	0.14, 0.79	5.45	11.1	4.13	1467
GaAs	(d/Z)	1.43	8500	400	0.067	0.074, 0.50	5.65	13.2	5.31	1238
GaN	(d/Z, W)	3.4	380	—	0.19	0.60	4.5	12.2	6.1	2530
GaSb	(d/Z)	0.7	5000	1000	0.042	0.06, 0.23	6.09	15.7	5.61	712
InP	(d/Z)	1.35	4000	100	0.077	0.089, 0.85	5.87	12.4	4.79	1070
InAs	(d/Z)	0.36	22600	200	0.023	0.025, 0.41	6.06	14.6	5.67	943
InSb	(d/Z)	0.18	10 ⁵	1700	0.014	0.015, 0.40	6.48	17.7	5.78	525
ZnS	(d/Z, W)	3.6	180	10	0.28	—	5.409	8.9	4.09	1650*
ZnSe	(d/Z)	2.7	600	28	0.14	0.60	5.671	9.2	5.65	1100*
ZnTe	(d/Z)	2.25	530	100	0.18	0.65	6.101	10.4	5.51	1238*
CdS	(d/W, Z)	2.42	250	15	0.21	0.80	4.137	8.9	4.82	1475
CdSe	(d/W)	1.73	800	—	0.13	0.45	4.30	10.2	5.81	1258
CdTe	(d/Z)	1.58	1050	100	0.10	0.37	6.482	10.2	6.20	1098
PbS	(i/H)	0.37	575	200	0.22	0.29	5.936	17.0	7.6	1119
PbSe	(i/H)	0.27	1500	1500	—	—	6.147	23.6	8.73	1081
PbTe	(i/H)	0.29	6000	4000	0.17	0.20	6.452	30	8.16	925

All values at 300 K.

*Vaporizes

p. 580

Homework #1.2 for Chapter 1: A2, A3, A4, 18



A2: The solid phase for C_{60} (molecular weight = $60 \times 12 = 720$ g/mole) has the crystal structure of *fcc* with a lattice constant of 14.17 \AA , please calculate its mass density.

A3: In a Bragg diffraction analysis, the order of diffraction $n = 2$, the wavelength $\lambda = 154\text{ pm}$, and the diffraction angle $\theta = 22.2^\circ$. Solve for the spacing between the crystal planes $d = ?$

A4: A Si crystal is to be pulled from the melt and doped with P. If the Si crystal weighs 275 kg, how many grams of P should be introduced to achieve $5.0 \times 10^{16}\text{ cm}^{-3}$ doping during the initial growth? What happened with the doping concentration on the final growth part?

TABLE 1 Equilibrium Segregation Coefficients for Dopants in Si

Dopant	k_0	Type	Dopant	k_0	Type
B	8×10^{-1}	p	As	3.0×10^{-1}	n
Al	2×10^{-3}	p	Sb	2.3×10^{-2}	n
Ga	8×10^{-3}	p	Te	2.0×10^{-4}	n
In	4×10^{-4}	p	Li	1.0×10^{-2}	n
O	1.25	n	Cu	4.0×10^{-4}	— ^a
C	7×10^{-2}	n	Au	2.5×10^{-5}	— ^a
P	0.35	n			

^aDeep-lying impurity level.

TABLE 2 Equilibrium Segregation Coefficients for Dopants in GaAs

Dopant	k_0	Type
Be	3	p
Mg	0.1	p
Zn	4×10^{-1}	p
C	0.8	n/p
Si	1.85×10^{-1}	n/p
Ge	2.8×10^{-2}	n/p
S	0.5	n
Se	5.0×10^{-1}	n
Sn	5.2×10^{-2}	n
Te	6.8×10^{-2}	n
Cr	1.03×10^{-4}	Semiinsulating
Fe	1.0×10^{-3}	Semiinsulating

- 1.18 Assuming that the lattice constant varies linearly with composition x for a ternary alloy (e.g., see the variation for InGaAs in Fig. 1-13),
(a) what composition of $\text{AlSb}_x\text{As}_{1-x}$ is lattice-matched to InP?
(b) What composition of $\text{In}_x\text{Ga}_{1-x}\text{P}$ is lattice-matched to GaAs?
(c) What is the band gap energy in each case?
- [Note: Such linear variations of crystal properties (e.g., lattice constant and band gap) with mole fraction in alloys is known as Vegard's law. A second-order polynomial or quadratic fit to the data is called the bowing parameter.]

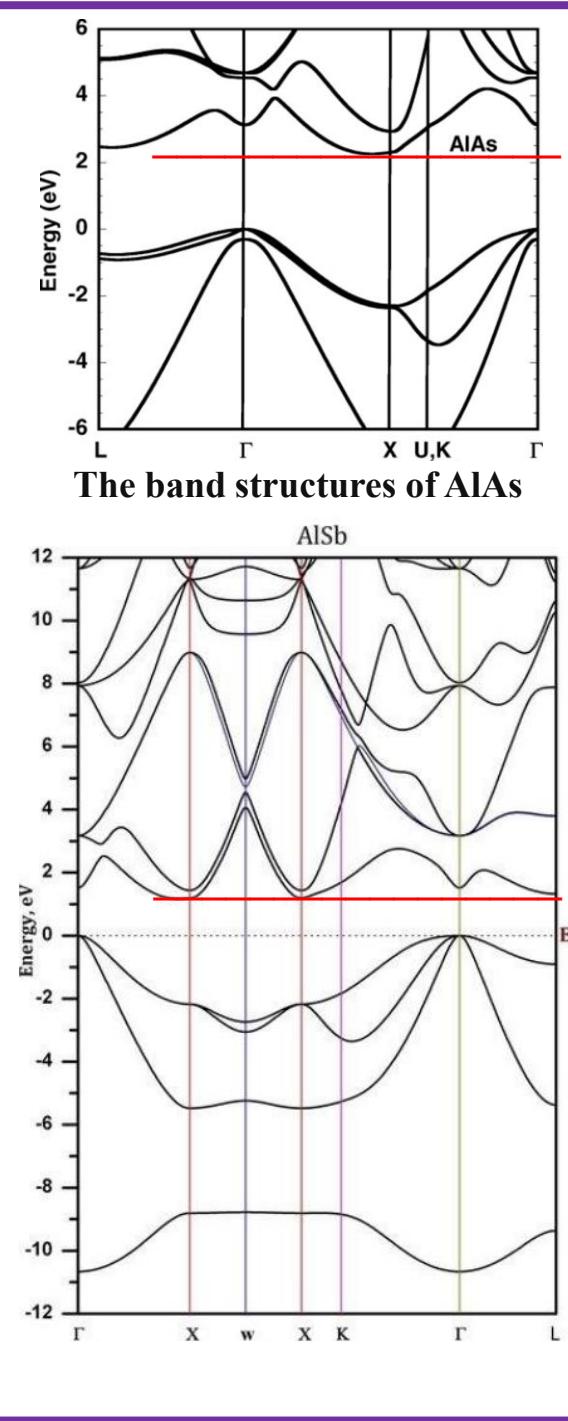
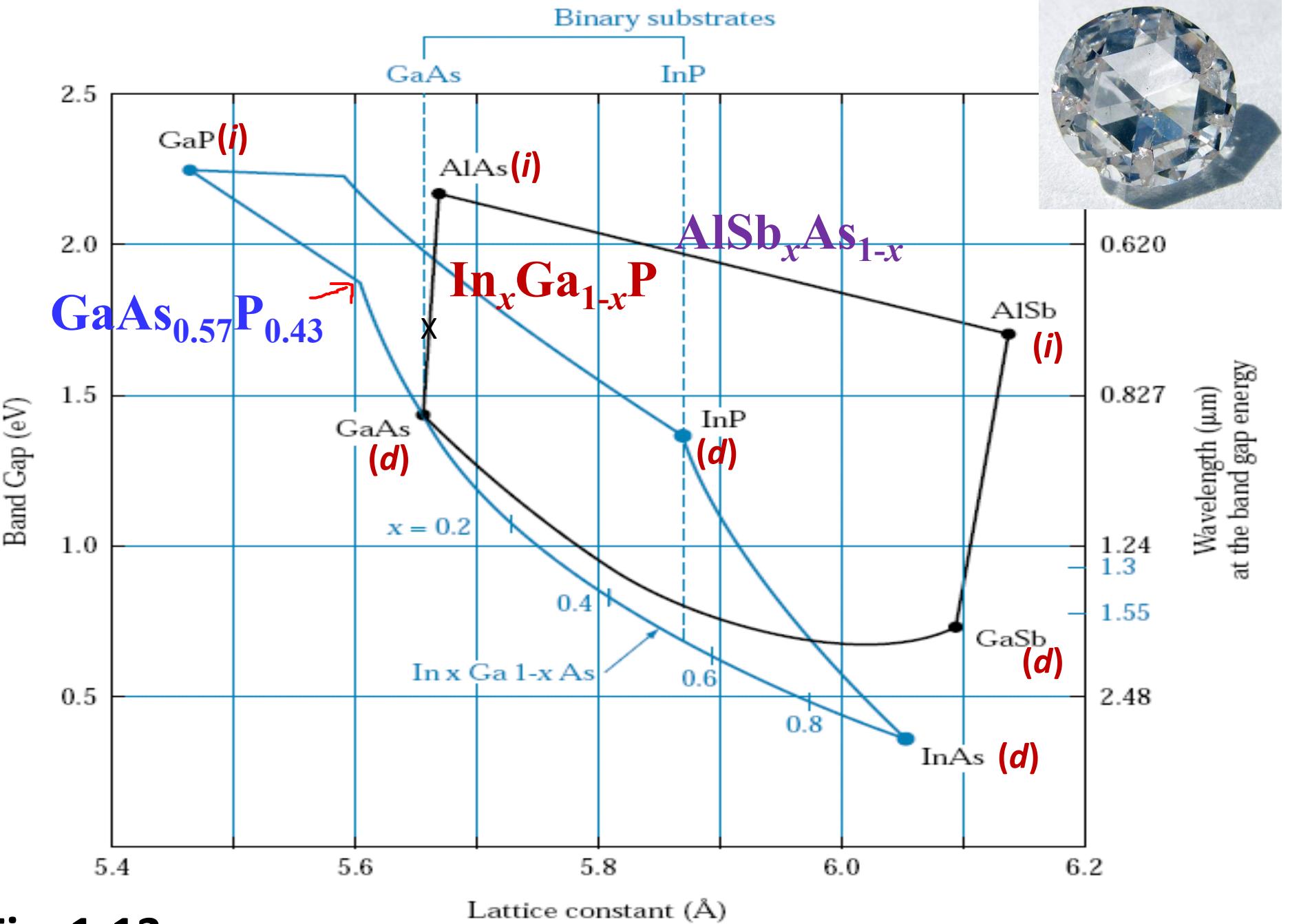


Fig. 1-13

		E_g (eV)	μ_n (cm ² /V-s)	μ_p (cm ² /V-s)	m_n^*/m_o (m_l, m_t)	m_p^*/m_o (m_{lh}, m_{hh})	a (Å)	ϵ_r	Density (g/cm ³)	Melting point (°C)
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Avogadro's number	$N_A = 6.02 \times 10^{23}$ molecules/mole
Boltzmann's constant	$k = 1.38 \times 10^{-23} \text{ J/K}$ $= 8.62 \times 10^{-5} \text{ eV/K}$
Electronic charge (magnitude)	$q = 1.60 \times 10^{-19} \text{ C}$
Electronic rest mass	$m_0 = 9.11 \times 10^{-31} \text{ kg}$
Permittivity of free space	$\epsilon_0 = 8.85 \times 10^{-14} \text{ F/cm}$ $= 8.85 \times 10^{-12} \text{ F/m}$
Planck's constant	$h = 6.63 \times 10^{-34} \text{ J-s}$ $= 4.14 \times 10^{-15} \text{ eV-s}$
Room temperature value of kT	$kT = 0.0259 \text{ eV}$
Speed of light	$c = 2.998 \times 10^{10} \text{ cm/s}$

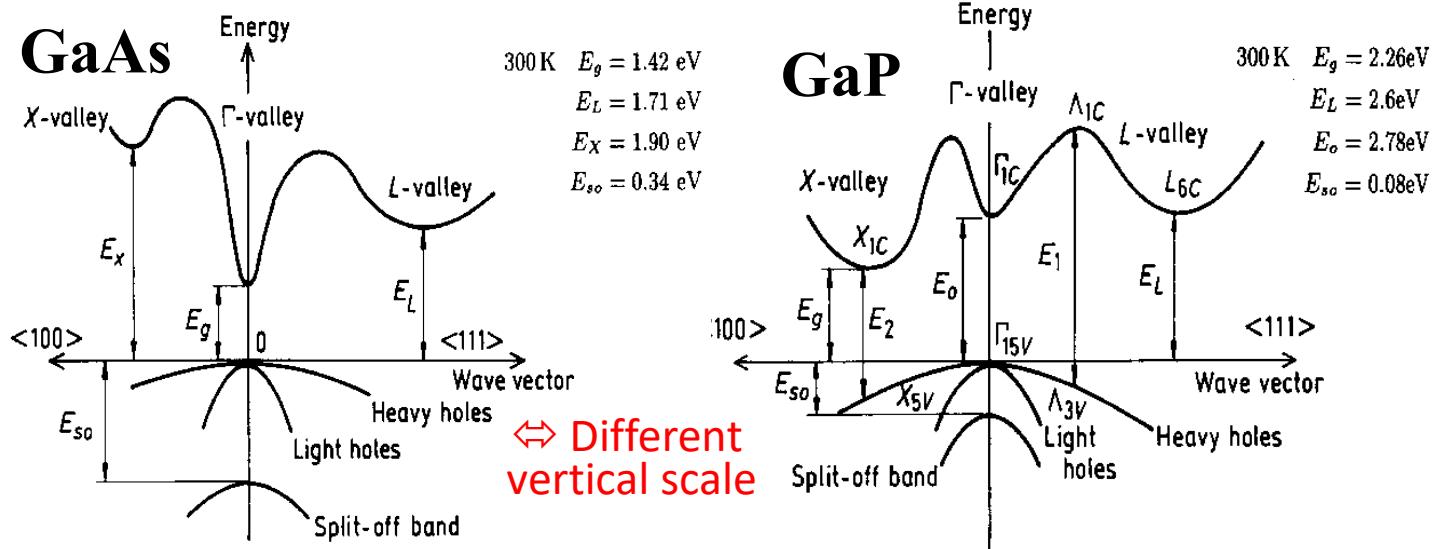
1 Å (angstrom) = 10^{-8} cm
 1 μm (micron) = 10^{-4} cm
 1 nm = 10 Å = 10^{-7} cm
 2.54 cm = 1 in.
 1 eV = 1.6×10^{-19} J

Prefixes:

milli-,	m-	= 10^{-3}
micro-,	μ-	= 10^{-6}
nano-,	n-	= 10^{-9}
pico-,	p-	= 10^{-12}
kilo-,	k-	= 10^3
mega-,	M-	= 10^6
giga-,	G-	= 10^9

A wavelength λ of 1 μm corresponds to a photon energy of 1.24 eV.

三元化合物半導體 $\text{GaAs}_{1-x}\text{P}_x$ 的 E_g 隨組成比 x 而變 => Bandgap engineering



<http://www.ioffe.ru/SVA/NSM/Semicond/GaAs/Figs/421.gif>

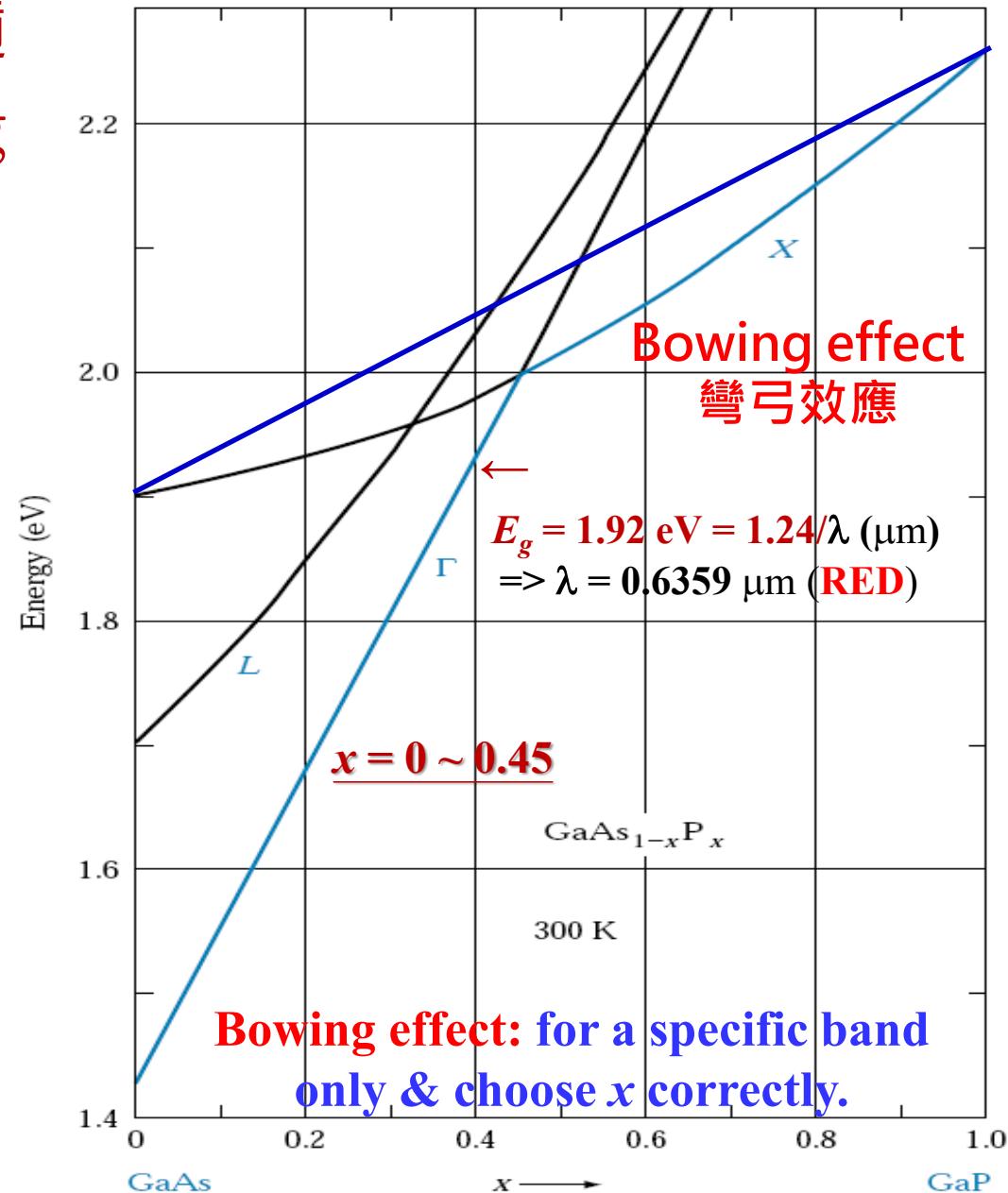
<https://www.ioffe.ru/SVA/NSM/Semicond/GaP/Figs/521.gif>

For the same Γ -band:

$$E_\Gamma(\text{GaAs}_{1-x}\text{P}_x) = [xE_\Gamma(\text{GaP}) + (1 - x)E_\Gamma(\text{GaAs})] - b_\Gamma x(1 - x)$$

For the same X-band:

$$E_X(\text{GaAs}_{1-x}\text{P}_x) = [xE_X(\text{GaP}) + (1 - x)E_X(\text{GaAs})] - b_X x(1 - x)$$



Bowing of the defect formation energy in semiconductor alloys, from *Phys. Rev. B* 87, 241201(R) (2013)

- Alloying different semiconductors is a popular approach to broaden the range of available material properties for specific applications. Considerable efforts have been made to understand **the compositional dependence of properties** of **isovalent $A_xB_{1-x}C$** (e.g., $\text{Al}_x\text{Ga}_{1-x}\text{As}$) semiconductor alloys. **Many alloy properties $P(A_xB_{1-x}C)$ can be described as a linear average of the corresponding quantities in two pure constituents and a quadratic term,**
- $$P(A_xB_{1-x}C) = [xP(AC) + (1 - x)P(BC)] - bx(1 - x),$$
 where **b** is the so-called **bowing coefficient**.
- Generally, **for isovalent alloys** with a **small chemical and size mismatch**, the **bowing coefficients are small constant numbers**; for alloys with a **large chemical and size mismatch**, the **bowing coefficients** could be **large and composition dependent**.