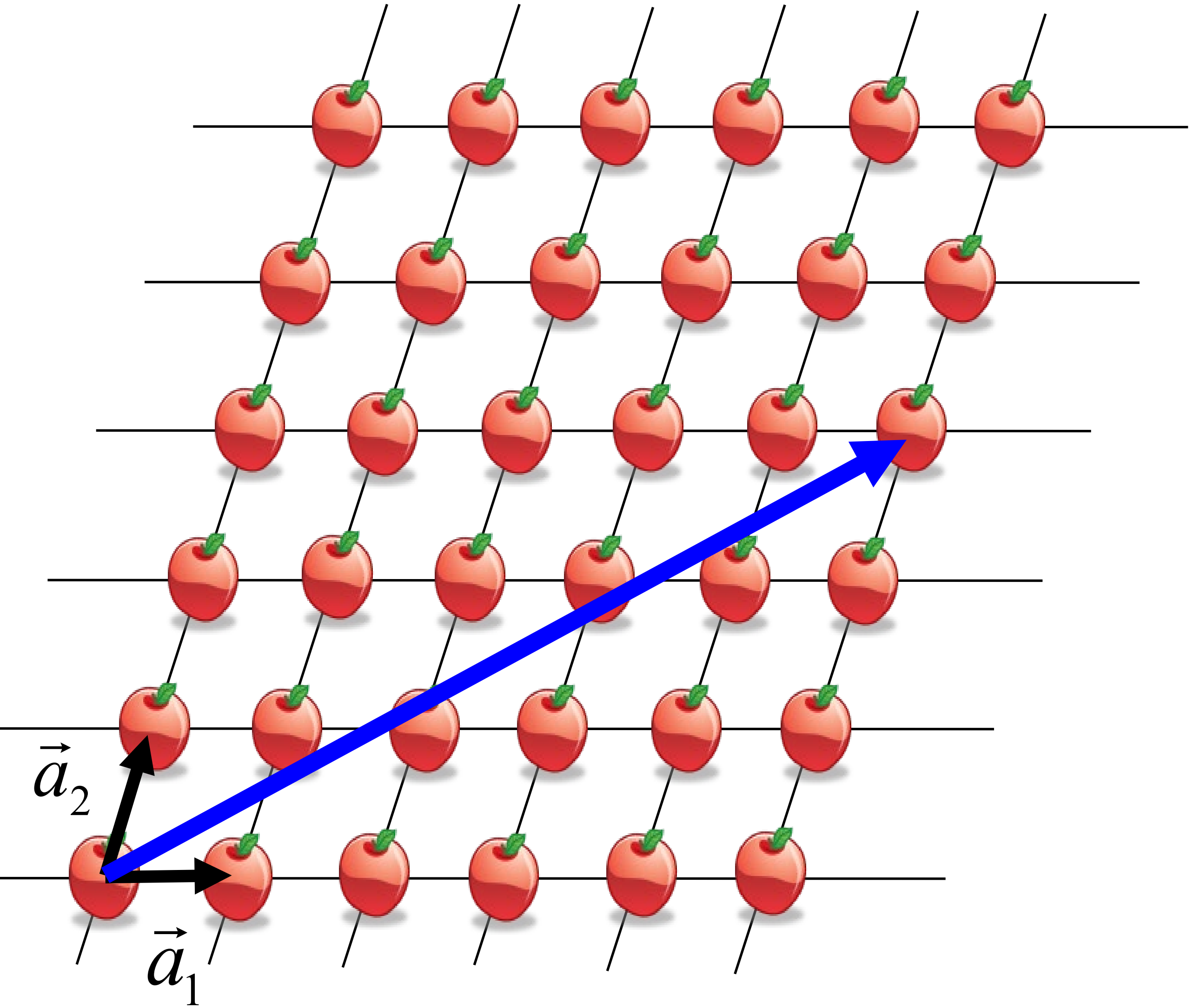
Lattice translation, primitive lattice vector



1. The lattice with the basis of single apple

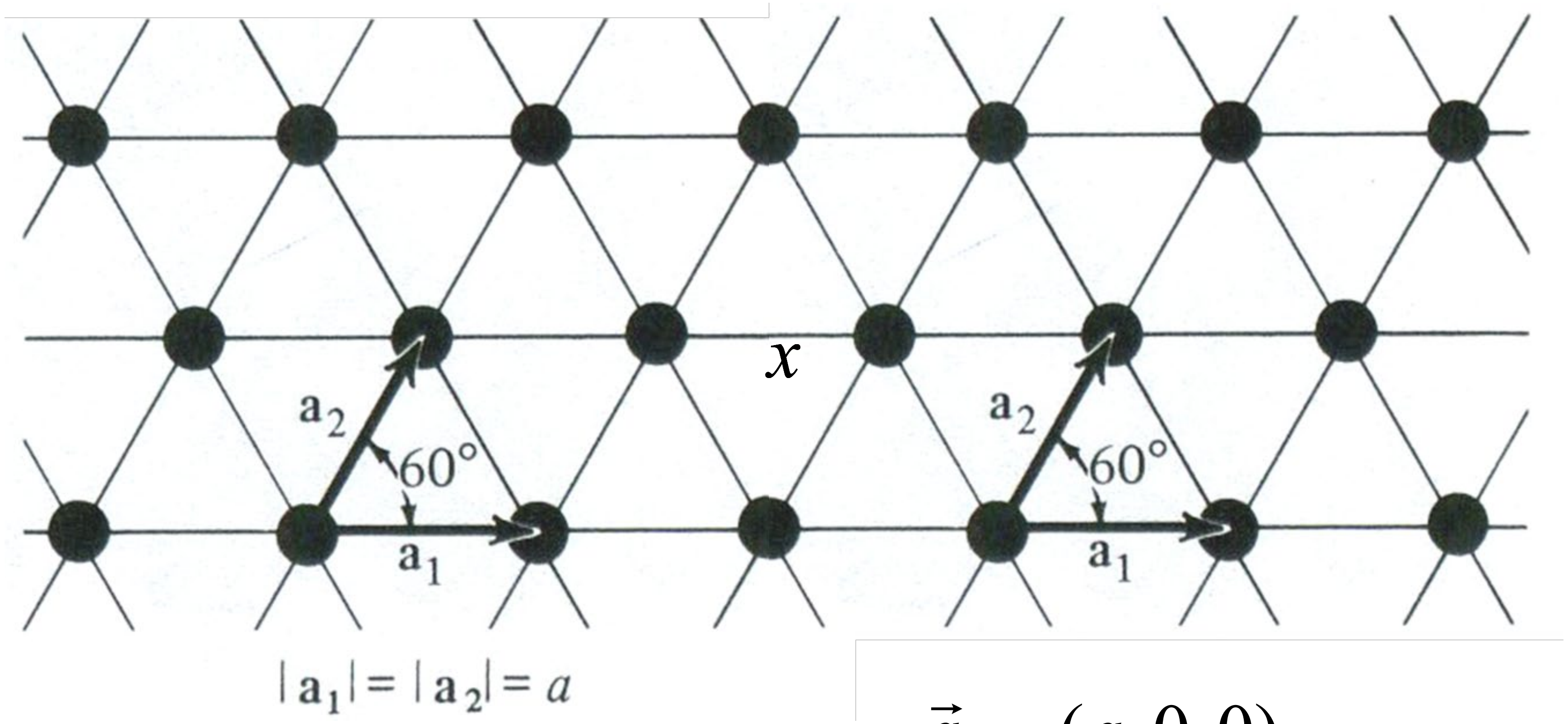
2. Lattice vector

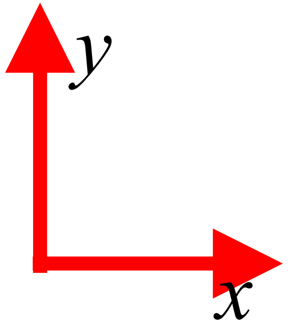
$$\vec{R} = n\vec{a}_1 + m\vec{a}_2 + l\vec{a}_3$$

3. Primitive lattice vector

$$\vec{a}_1 \ , \ \vec{a}_2 \ , \ \vec{a}_3$$

Triangular lattice

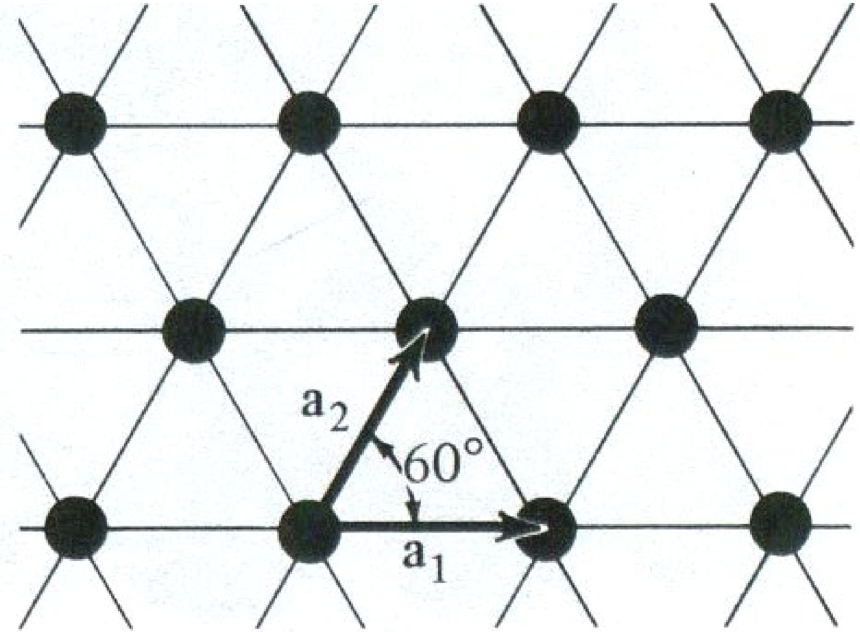




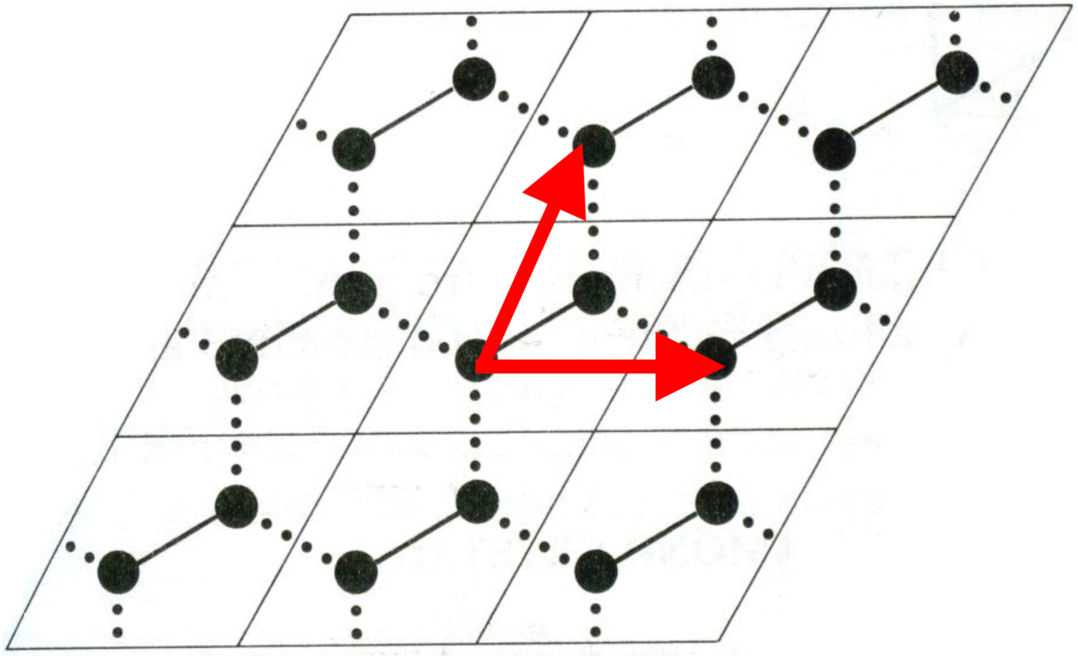
$$\vec{a}_1 = (a, 0, 0)$$

$$\vec{a}_2 = (\frac{1}{2}a, \frac{\sqrt{3}}{2}a, 0)$$

Honeycomb = triangular lattice with two basis



$|\mathbf{a}_1| = |\mathbf{a}_2| = a$



For a lattice defined by $\vec{a}_1, \vec{a}_2, \vec{a}_3$

1. Unit cell volume

$$V = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$$

2. The primitive lattice vectors for the reciprocal lattice

$$\vec{b}_1 = \frac{2\pi}{V}(\vec{a}_2 \times \vec{a}_3)\ ,\ \vec{b}_2 = \frac{2\pi}{V}(\vec{a}_3 \times \vec{a}_1)\ ,\ \vec{b}_3 = \frac{2\pi}{V}(\vec{a}_1 \times \vec{a}_2)$$

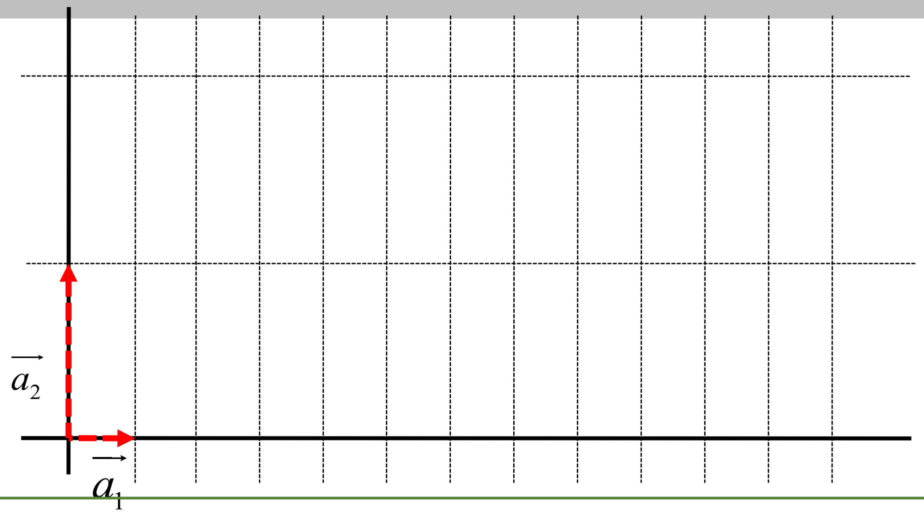
3. Show that

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{i,j}$$

$$\vec{a}_1 \cdot \vec{b}_1 = ???$$

$$\vec{a}_1 \cdot \vec{b}_2 = ???$$

Example: an orthorhombic lattice

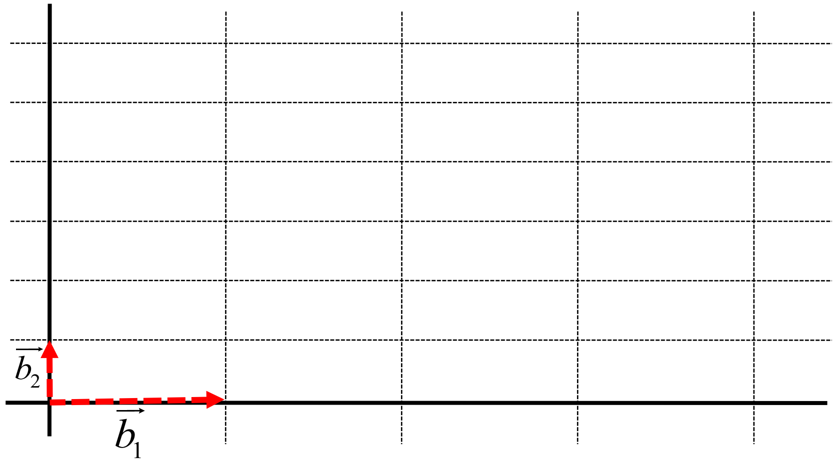


$$\begin{cases} \vec{a}_1 = a\hat{x} \\ \vec{a}_2 = 3a\hat{y} \\ \vec{a}_3 = a\hat{z} \end{cases}$$

$$V = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = 3a^3$$

$$\vec{b}_1 = 2\pi \frac{3a^2}{3a^3}, \quad \vec{b}_2 = 2\pi \frac{a^2}{3a^3}, \quad \vec{b}_3 = 2\pi \frac{3a^2}{3a^3}$$

$$\vec{b}_1 = \frac{2\pi}{a}\hat{x}, \quad \vec{b}_2 = \frac{2\pi}{3a}\hat{y}, \quad \vec{b}_3 = \frac{2\pi}{a}\hat{z}$$



$$\vec{a}_1 \cdot \vec{b}_1 = 2\pi \qquad \vec{a}_1 \cdot \vec{b}_3 = 0$$

$$\vec{a}_1 \cdot \vec{b}_2 = 0 \qquad \vec{a}_2 \cdot \vec{b}_2 = 2\pi$$

$$\vdots$$

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$$

Direct Lattice	Reciprocal Lattice
$\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$	$\{\vec{b}_1, \vec{b}_2, \vec{b}_3\}$
$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$	$\vec{G} = l_1\vec{b}_1 + l_2\vec{b}_2 + l_3\vec{b}_3$

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$$

$$\vec{R} \cdot \vec{G} = 2\pi\,(n_1 l_1 + n_2 l_2 + n_3 l_3)$$

$$= 2\pi \times (\text{ integer})$$

(a lattice vector) • (a Reciprocal lattice vector) = integer multiple of 2π

We have three vectors

$$\rho(\vec{r}') = \rho(\vec{r}' + \vec{R})$$

1. Lattice vectors

$$\vec{R} = n\vec{a}_1 + l\vec{a}_2 + m\vec{a}_3$$

2. Reciprocal Lattice vectors

$$\vec{G} = n\vec{b}_1 + l\vec{b}_2 + m\vec{b}_3$$

Fourier transformation,,

Fourier **wave vector** = Reciprocal Lattice vector

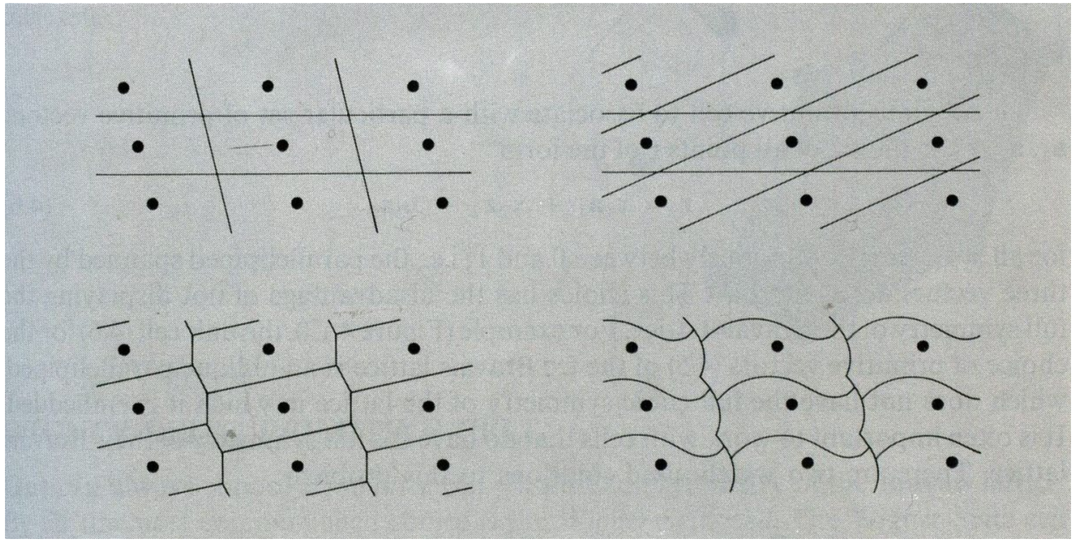
3. Bloch vectors

$$\vec{k} = \alpha\vec{b}_1 + \beta\vec{b}_2 + \gamma\vec{b}_3$$

Lattice translation, primitive lattice vector

$$\vec{R} = n\vec{a}_1 + m\vec{a}_2 + l\vec{a}_3$$

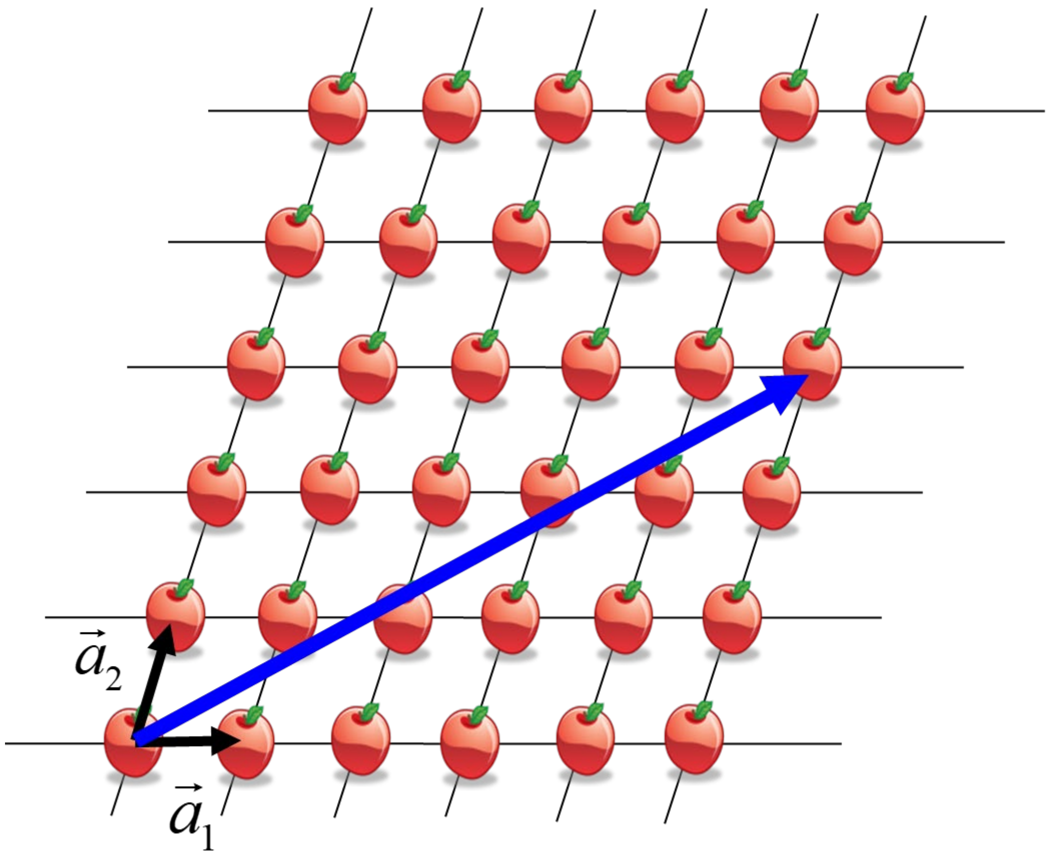
Primitive unit cell, through the lattice translations, can fill out the space without overlap and without void.



$$V = \vec{a} \cdot (\vec{b} \times \vec{c})$$

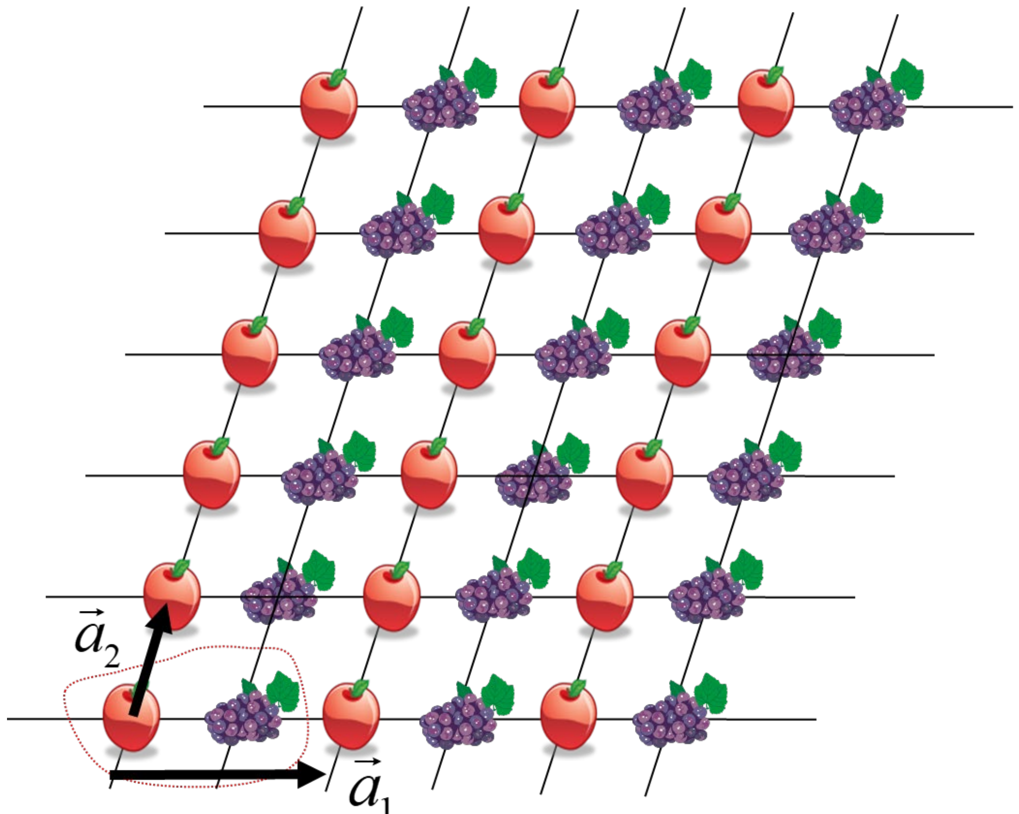
Volume of unit-cell is defined above, but the shape of unit-cell can be arbitrary.

The basis of the lattice

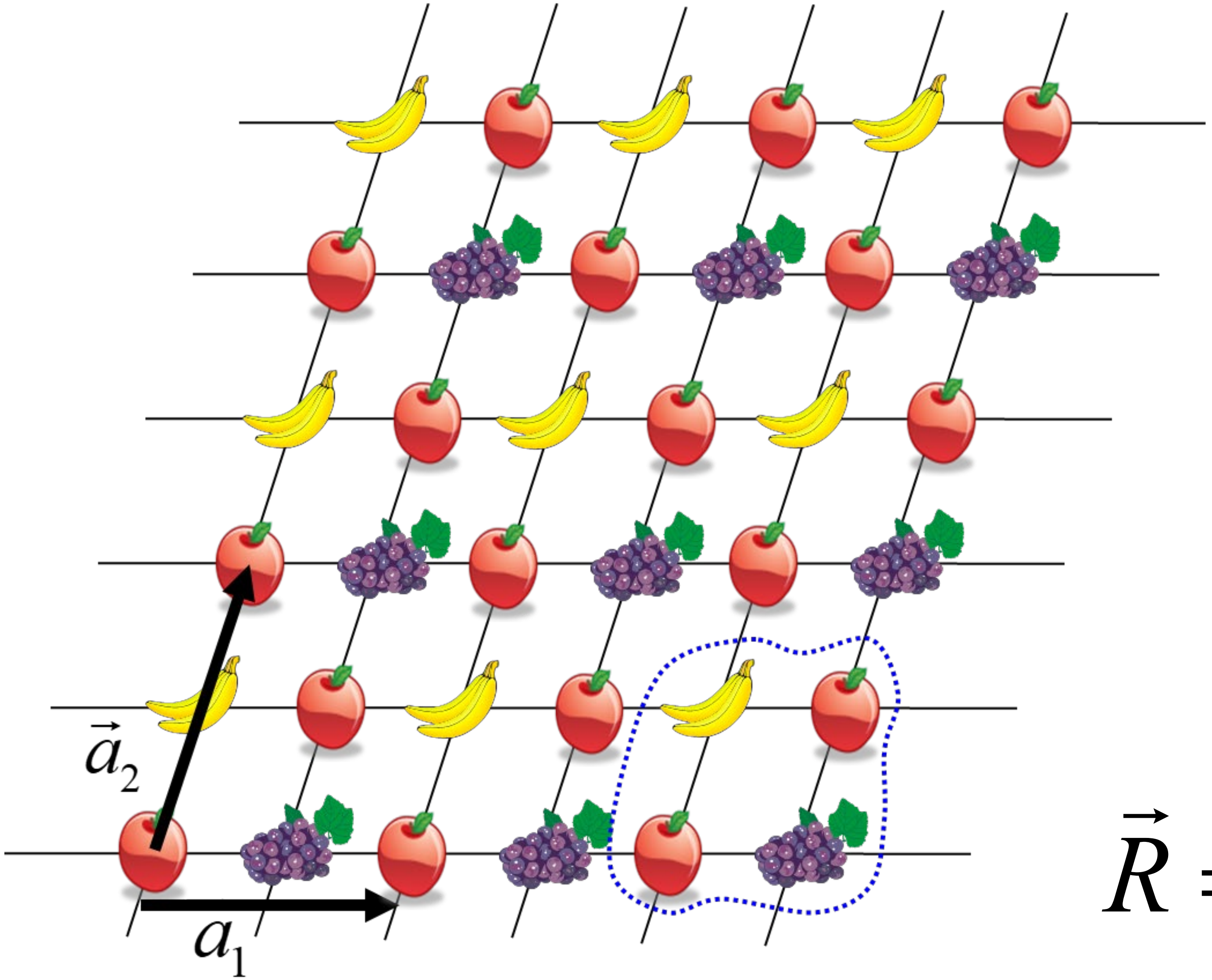


Single apple

One apple and one grape

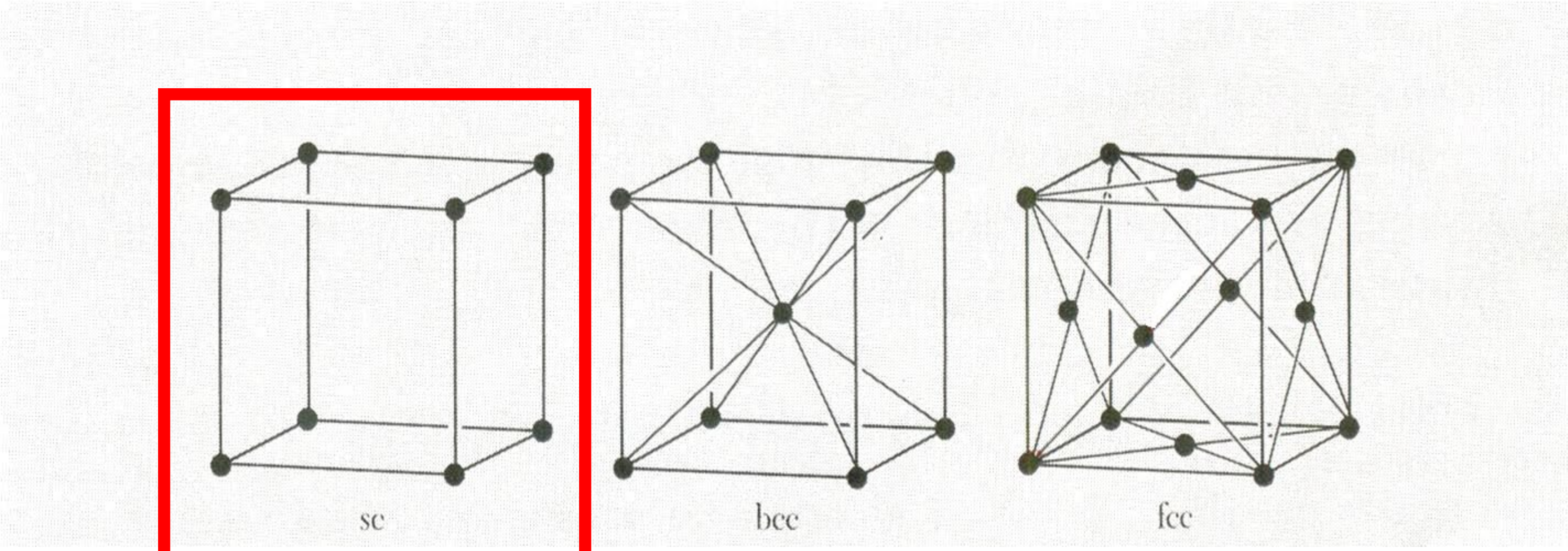


The basis of the lattice



$$\vec{R} = n\vec{a}_1 + m\vec{a}_2$$

Cubic lattice

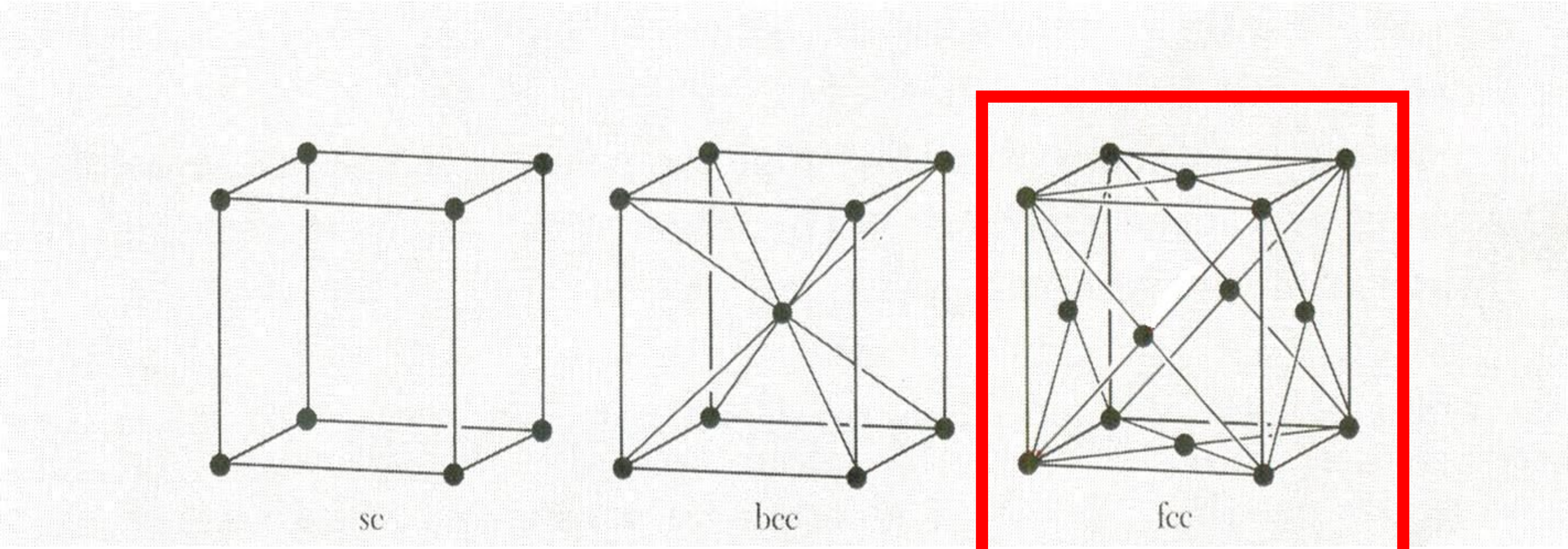


(a) (b) (c)

(a) Simple Cubic Bravais lattice with the primitive cell of

$$\overrightarrow{a_1} = a\hat{i},\ \overrightarrow{a_2} = a\hat{j},\ \overrightarrow{a_3} = a\hat{k}$$

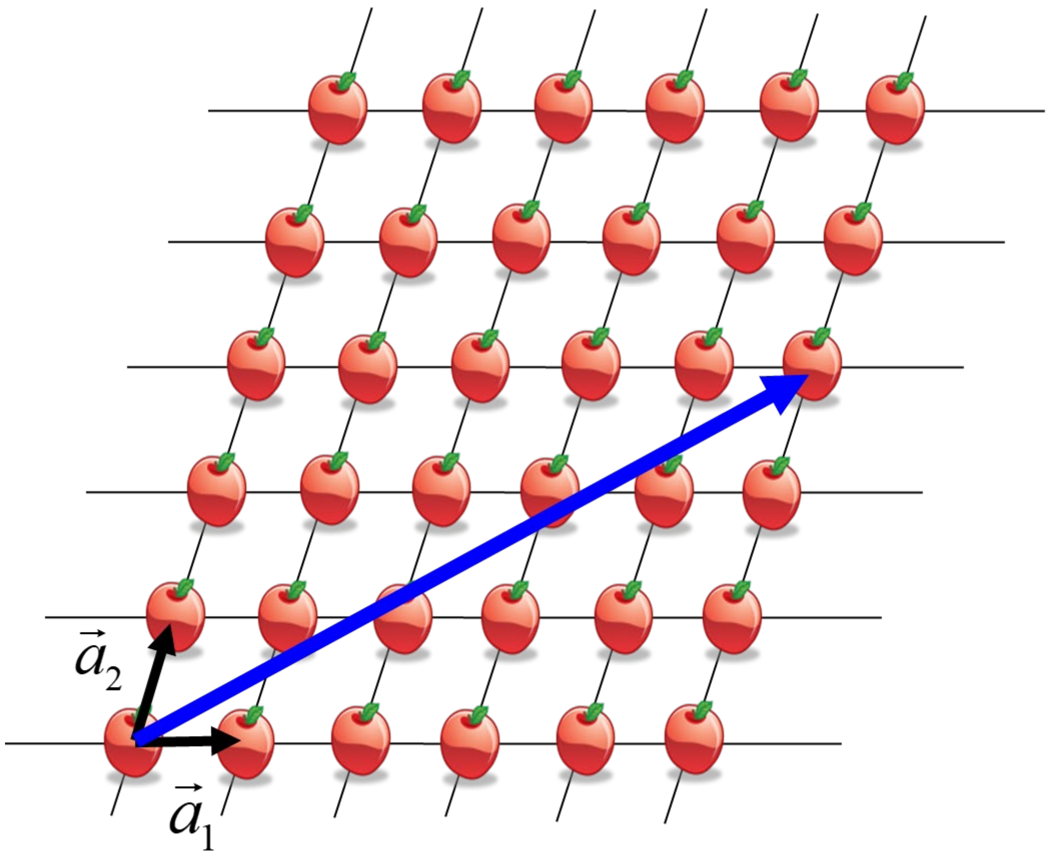
How many lattice points in the unit cell ?



(a) (b) (c)

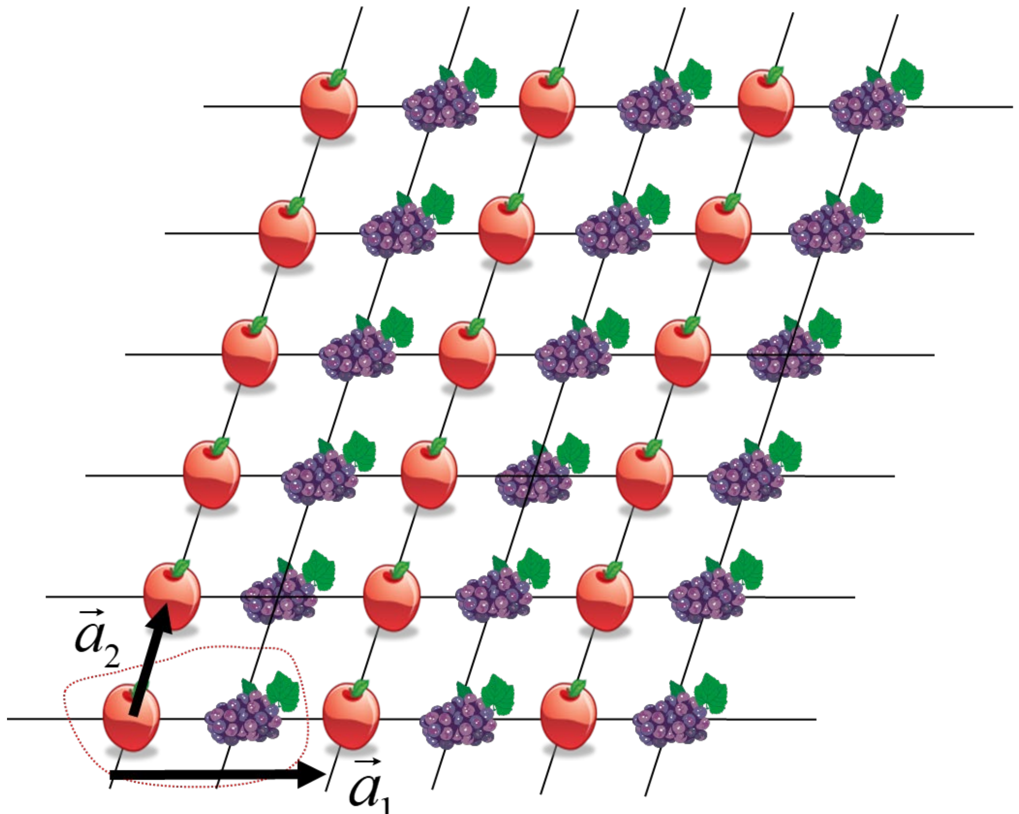
What is the lattice for the structure (c) ?

How many lattice points in the unit cell ?

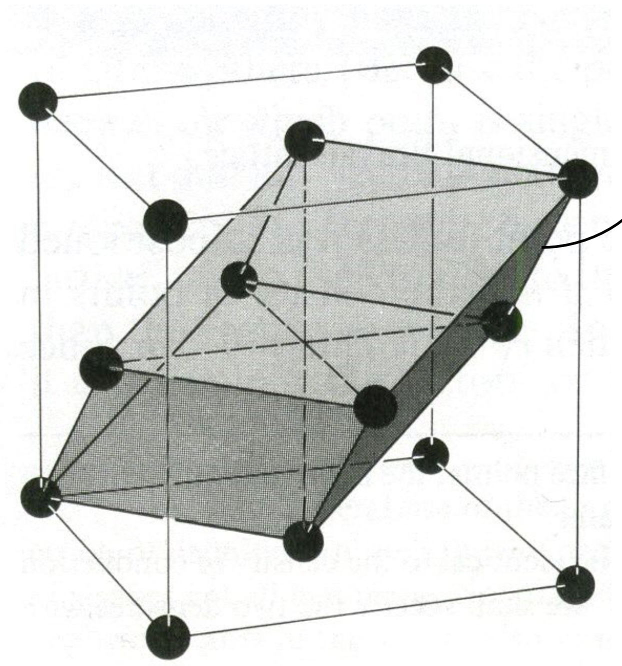


Single apple

One apple and one grape



Face-centered Cubic

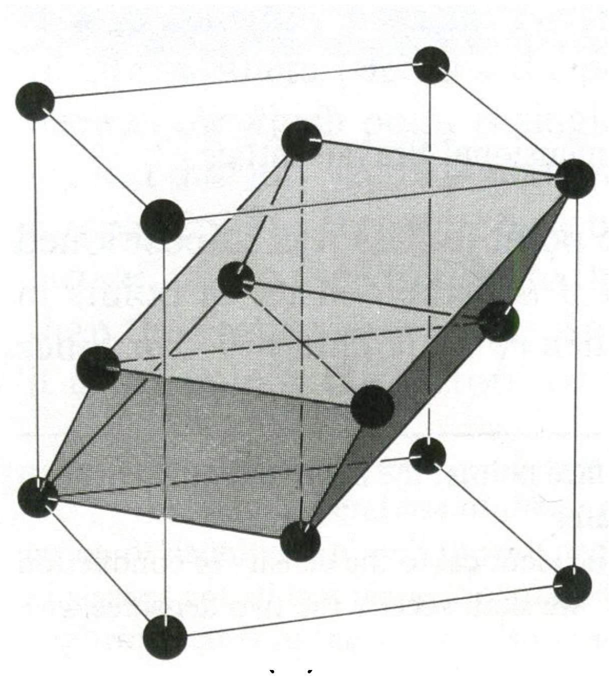


$$\left\{ \begin{aligned} \vec{a}_1 &= \frac{a}{2}(\hat{i}+\hat{j}) \\ \vec{a}_2 &= \frac{a}{2}(\hat{j}+\hat{k}) \\ \vec{a}_3 &= \frac{a}{2}(\hat{k}+\hat{i}) \end{aligned} \right\}$$

FCC Bravais lattice,

Remember it has one spherical symmetric object in the unit cell

Face-centered Cubic

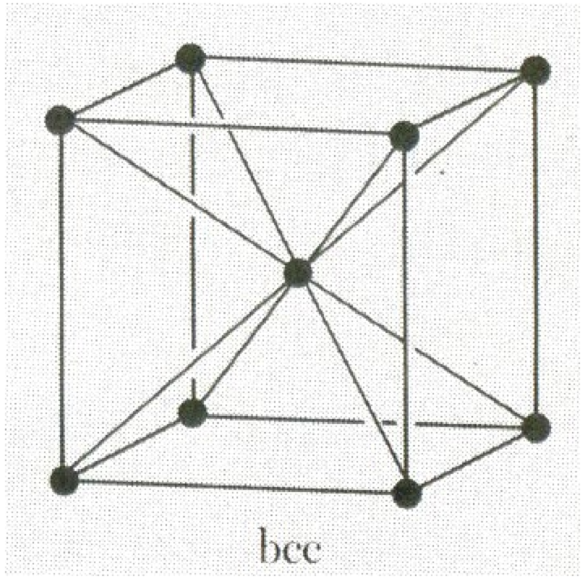


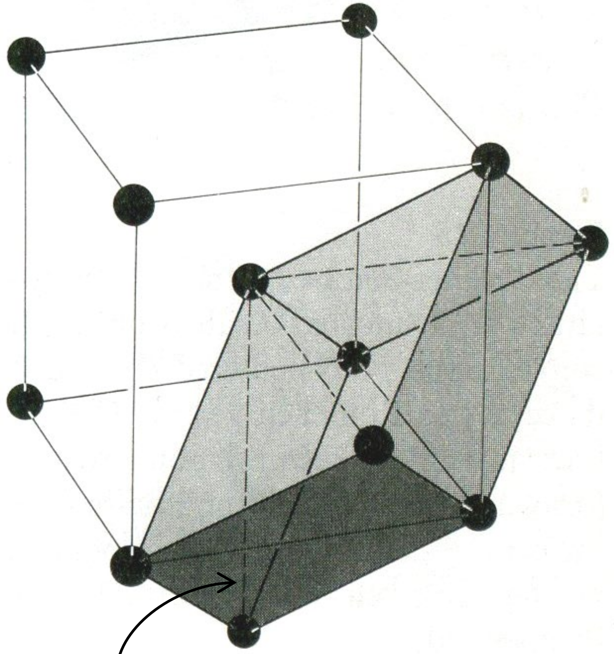
$$\overrightarrow{a_1} = a\hat{i}, \ \overrightarrow{a_2} = a\hat{j}, \ \overrightarrow{a_3} = a\hat{k}$$

But the FCC structure can be described with a simple cubit lattice ?

How many atoms are there in this SC cell ?

Body-centered cubic



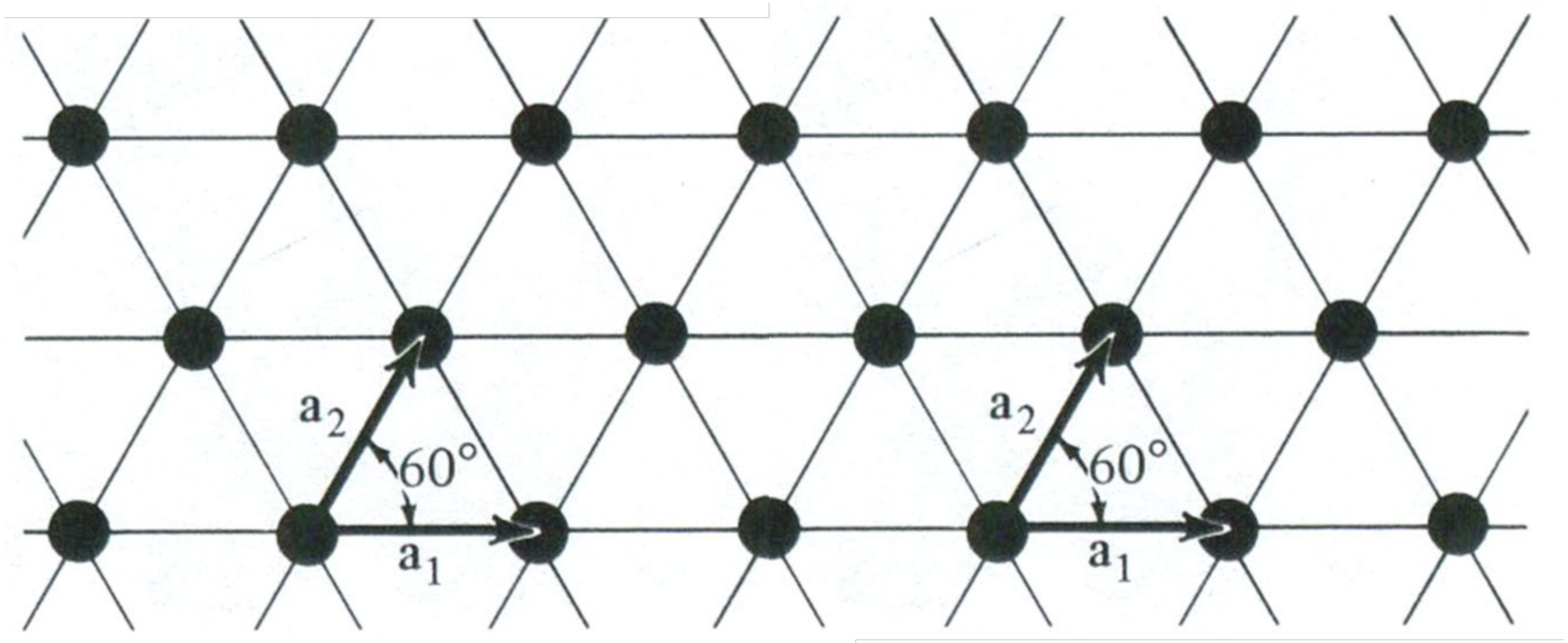


$$\overrightarrow{a_1} = \frac{a}{2}(\hat{y} + \hat{z} - \hat{x})$$

$$\overrightarrow{a_2} = \frac{a}{2}(\hat{z} + \hat{x} - \hat{y})$$

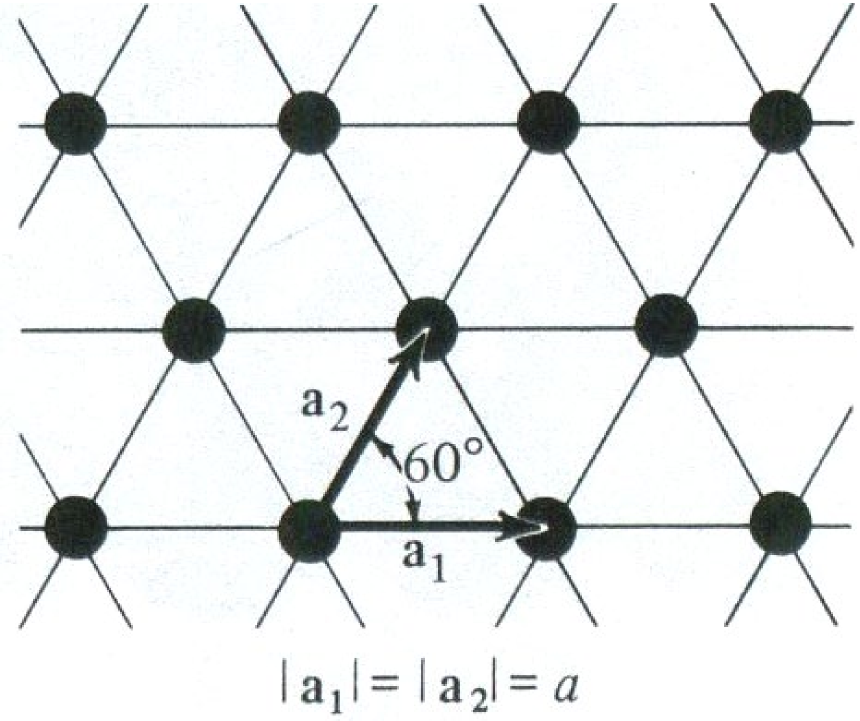
$$\overrightarrow{a_3} = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$

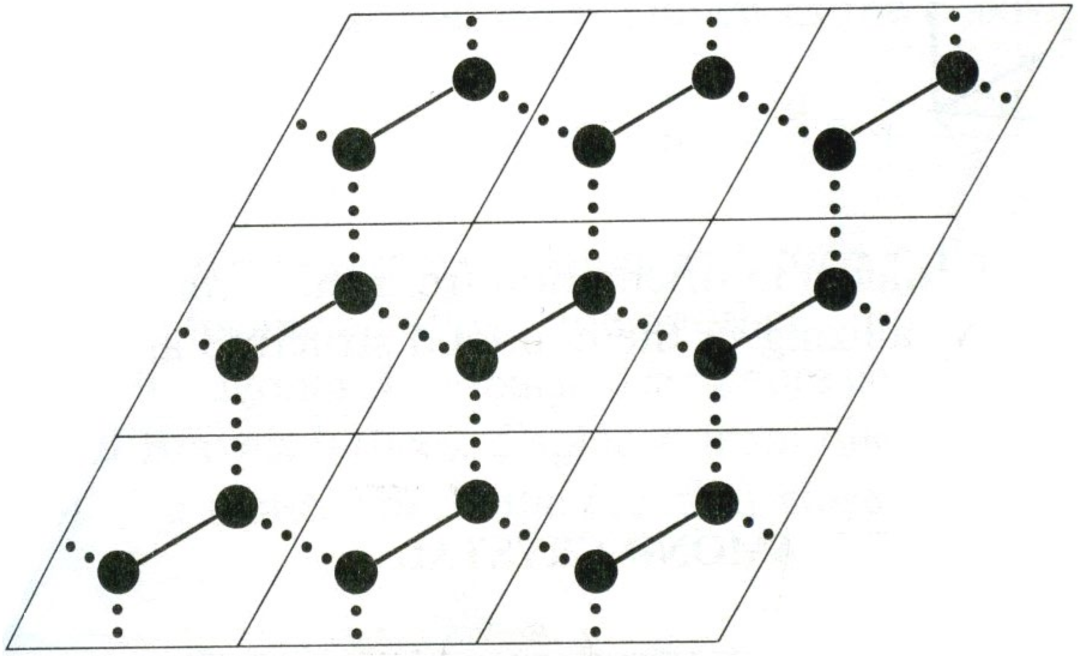
Triangular lattice



$|\mathbf{a}_1| = |\mathbf{a}_2| = a$

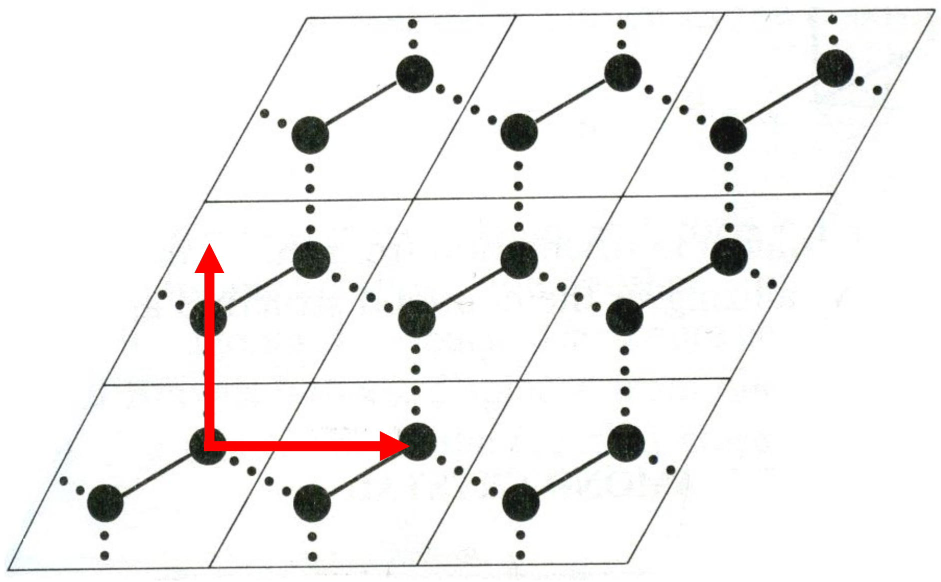
Honey Com

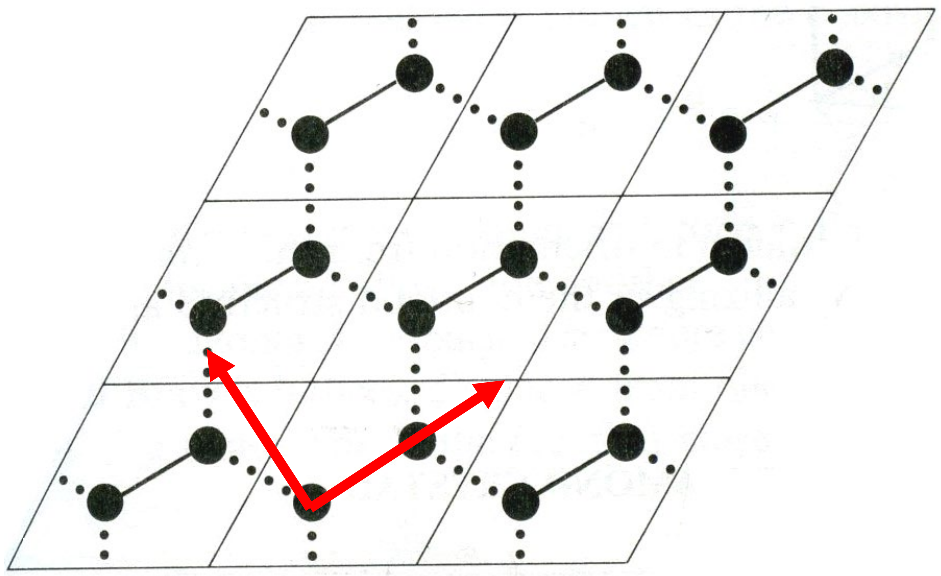




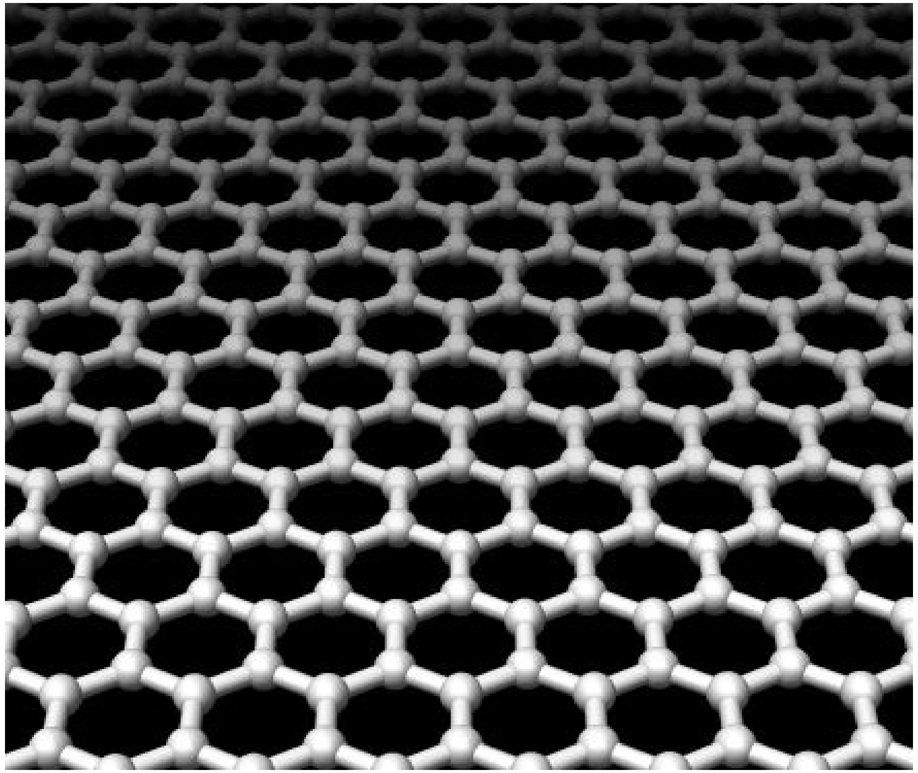
Example,

Choosing the following two set of coordinate, express the components of lattice vector and basis vector.





Honey Comb structure

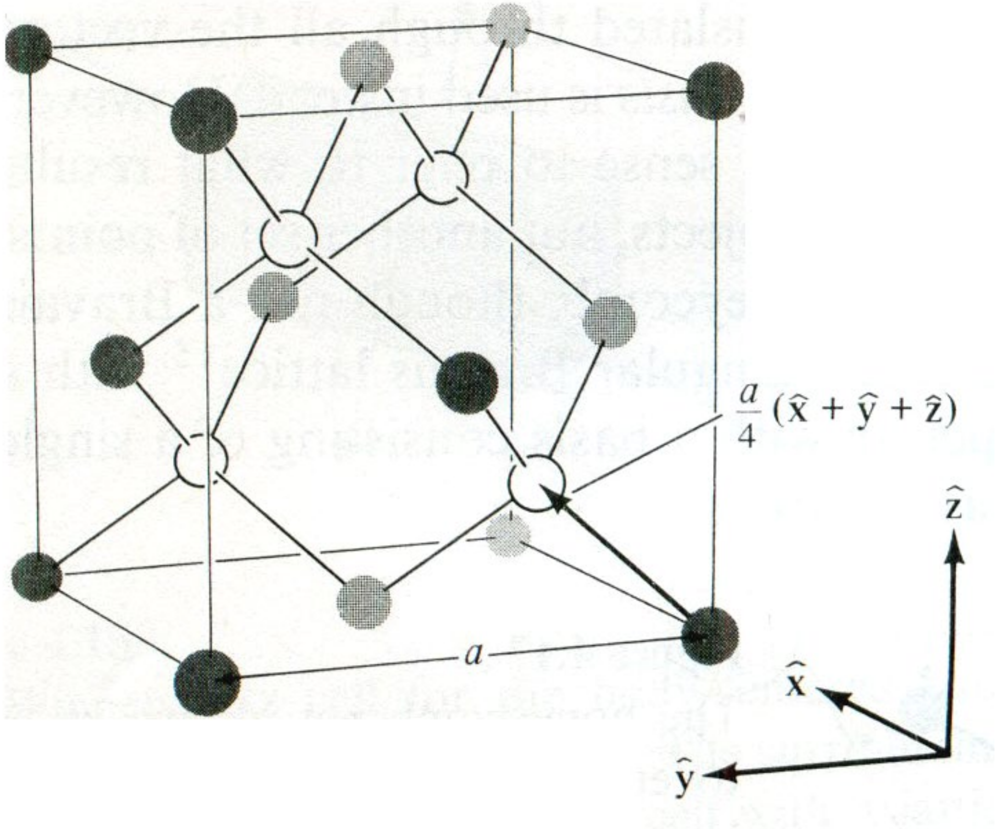


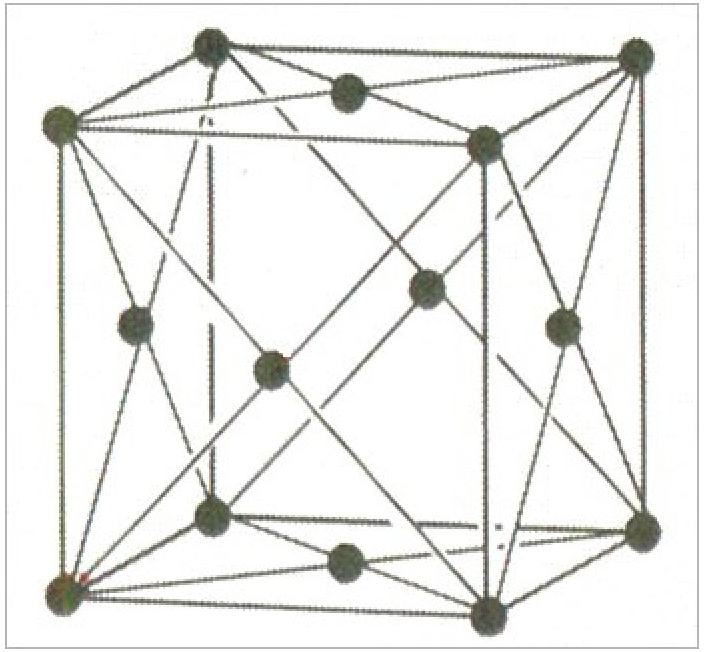
Semiconductor

1B	2B	3A	4A	5A	6A	7A	NOBLE ELEMENTS
							HELIUM 4.0026 0.179 He 2 $1s^2$ 3.57 HEX 1.633 ~1.0 (26 Atm) 26^{LT}
		BORON 10.81 2.34 B 5 $1s^2 2s^2 2p^1$ 8.73 TET 0.576 2600 1250	CARBON 12.01 2.26 C 6 $1s^2 2s^2 2p^2$ 3.57 DIA (4300) 1860	NITROGEN 14.007 1.03 N 7 $1s^2 2s^2 2p^3$ 4.039 HEX 1.651 63.3 (β) 79^{LT}	OXYGEN 15.999 1.43 O 8 $1s^2 2s^2 2p^4$ 6.83 CUB 54.7 (γ) 46^{LT}	FLUORINE 18.998 1.97 (α) F 9 $1s^2 2s^2 2p^5$ MCL 53.5	NEON 20.18 1.56 Ne 10 $1s^2 2s^2 2p^6$ 4.43 FCC 24.5 63
		ALUMINUM 26.982 2.70 Al 13 [Ne] $3s^2 3p^1$ 4.05 FCC 933 394	SILICON 28.086 2.33 Si 14 [Ne] $3s^2 3p^2$ 5.43 DIA 1683 625	PHOSPHORUS 30.974 1.82 (white) P 15 [Ne] $3s^2 3p^3$ 7.17 CUB 317.3	SULFUR 32.064 2.07 S 16 [Ne] $3s^2 3p^4$ 10.47 ORC 2.339 1.229 386	CHLORINE 35.453 2.09 Cl 17 [Ne] $3s^2 3p^5$ 6.24 ORC 1.324 0.718 172.2	ARGON 39.948 1.78 Ar 18 [Ne] $3s^2 3p^6$ 5.26 FCC 83.9 85
COPPER 63.55 8.96 Cu 29 [Ar] $3d^{10} 4s^1$ 3.61 FCC 1356 315	ZINC 65.38 7.14 Zn 30 [Ar] $3d^{10} 4s^2$ 2.66 HEX 1.856 693 234	GALLIUM 69.72 5.91 Ga 31 [Ar] $3d^{10} 4s^2 4p^1$ 4.51 ORC 1.695 1.001 303 240	GERMANIUM 72.59 5.32 Ge 32 [Ar] $3d^{10} 4s^2 4p^2$ 5.66 DIA 1211 360	ARSENIC 74.922 5.72 As 33 [Ar] $3d^{10} 4s^2 4p^3$ 4.13 RHL 54°10′ 1090 285	SELENIUM 78.96 4.79 Se 34 [Ar] $3d^{10} 4s^2 4p^4$ 4.36 HEX 1.136 490 150^{LT}	BROMINE 79.91 4.10 Br 35 [Ar] $3d^{10} 4s^2 4p^5$ 6.67 ORC 1.307 0.672 266	KRYPTON 83.80 3.07 Kr 36 [Ar] $3d^{10} 4s^2 4p^6$ 5.72 FCC 116.5 73^{LT}
SILVER 107.87 10.5 Ag 47 [Kr] $4d^{10} 5s^1$ 4.09 FCC 1234 215	CADMIUM 112.40 8.65 Cd 48 [Kr] $4d^{10} 5s^2$ 2.98 HEX 1.886 594 120	INDIUM 114.82 7.31 In 49 [Kr] $4d^{10} 5s^2 5p^1$ 4.59 TET 1.076 429.8 129	TIN 118.69 7.30 Sn 50 [Kr] $4d^{10} 5s^2 5p^2$ 5.82 TET 0.546 505 170	ANTIMONY 121.75 6.62 Sb 51 [Kr] $4d^{10} 5s^2 5p^3$ 4.51 RHL 57°6′ 904 200	TELLURIUM 127.60 6.24 Te 52 [Kr] $4d^{10} 5s^2 5p^4$ 4.45 HEX 1.330 723 139^{LT}	IODINE 126.90 4.94 I 53 [Kr] $4d^{10} 5s^2 5p^5$ 7.27 ORC 1.347 0.659 387	XENON 131.30 3.77 Xe 54 [Kr] $4d^{10} 5s^2 5p^6$ 6.20 FCC 161.3 55^{LT}
GOLD 196.97 19.3 Au 79 [Xe] $4f^{14} 5d^{10} 6s^1$ 4.08 FCC 1337 170	MERCURY 200.59 13.6 Hg 80 [Xe] $4f^{14} 5d^{10} 6s^2$ 2.99 RHL 70°45′ 234.3 100	THALLIUM 204.37 11.85 Tl 81 [Xe] $4f^{14} 5d^{10} 6s^2 6p^1$ 3.46 HEX 1.599 577 96	LEAD 207.19 11.4 Pb 82 [Xe] $4f^{14} 5d^{10} 6s^2 6p^2$ 4.95 FCC 601 88	BISMUTH 208.98 9.8 Bi 83 [Xe] $4f^{14} 5d^{10} 6s^2 6p^3$ 4.75 RHL 57°14′ 544.5 120	POLONIUM 210 9.4 Po 84 [Xe] $4f^{14} 5d^{10} 6s^2 6p^4$ 3.35 SC 527	ASTATINE 210 At 85 [Xe] $4f^{14} 5d^{10} 6s^2 6p^5$ (575)	RADON 222 (4.4) Rn 86 [Xe] $4f^{14} 5d^{10} 6s^2 6p^6$ (FCC) (202)

GADOLINIUM 157.25 8.23 Gd 64 [Xe] $4f^7 5d^1 6s^2$ 3.64 HEX 1.588 1585 176^{LT}	TERBIUM 158.92 8.54 Tb 65 [Xe] $4f^9 5d^0 6s^2$ 3.60 HEX 1.581 1633 188^{LT}	DYSPROSIUM 162.50 8.78 Dy 66 [Xe] $4f^{10} 5d^0 6s^2$ 3.59 HEX 1.573 1680 186^{LT}	HOLMIUM 164.93 9.05 Ho 67 [Xe] $4f^{11} 5d^0 6s^2$ 3.58 HEX 1.570 1743 191^{LT}	ERBIUM 167.26 9.37 Er 68 [Xe] $4f^{12} 5d^0 6s^2$ 3.56 HEX 1.570 1795 195^{LT}	THULIUM 168.93 9.31 Tm 69 [Xe] $4f^{13} 5d^0 6s^2$ 3.54 HEX 1.570 1818 200^{LT}	YTTERBIUM 173.04 6.97 Yb 70 [Xe] $4f^{14} 5d^0 6s^2$ 5.49 FCC 1097 118^{LT}	LUTETIUM 174.97 9.84 Lu 71 [Xe] $4f^{14} 5d^1 6s^2$ 3.51 HEX 1.585 1929 207^{LT}
CURIUM 247 Cm 96 [Rn] $5f^7 6d^1 7s^2$ 1600	BERKELIUM 247 Bk 97 [Rn] $5f^7 6d^2 7s^2$	CALIFORNIUM 251 Cf 98 [Rn] $5f^9 6d^1 7s^2$	EINSTEINIUM 254 Es 99	FERMIUM 257 Fm 100	MENDELEVIUM 256 Md 101	NOBELIUM 254 No 102	LAWRENCIUM 257 Lw 103

Diamond structure = FCC with two basis





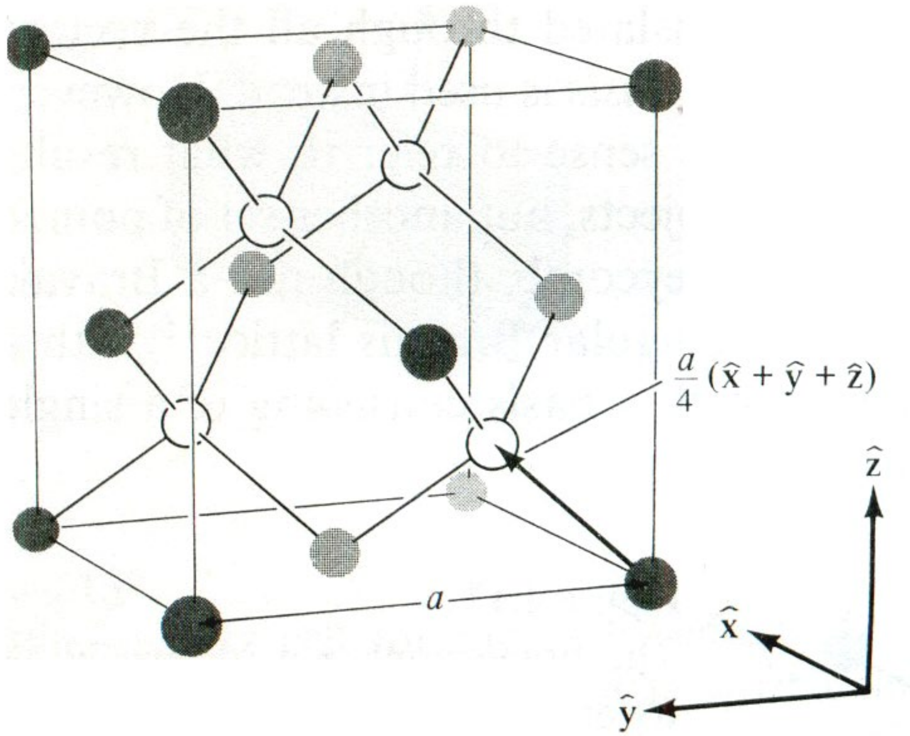
FCC

Diamond structure = FCC with two basis

Using an appropriate set of coordinate, express the coordinate vectors for the basis atoms and lattice vector ?

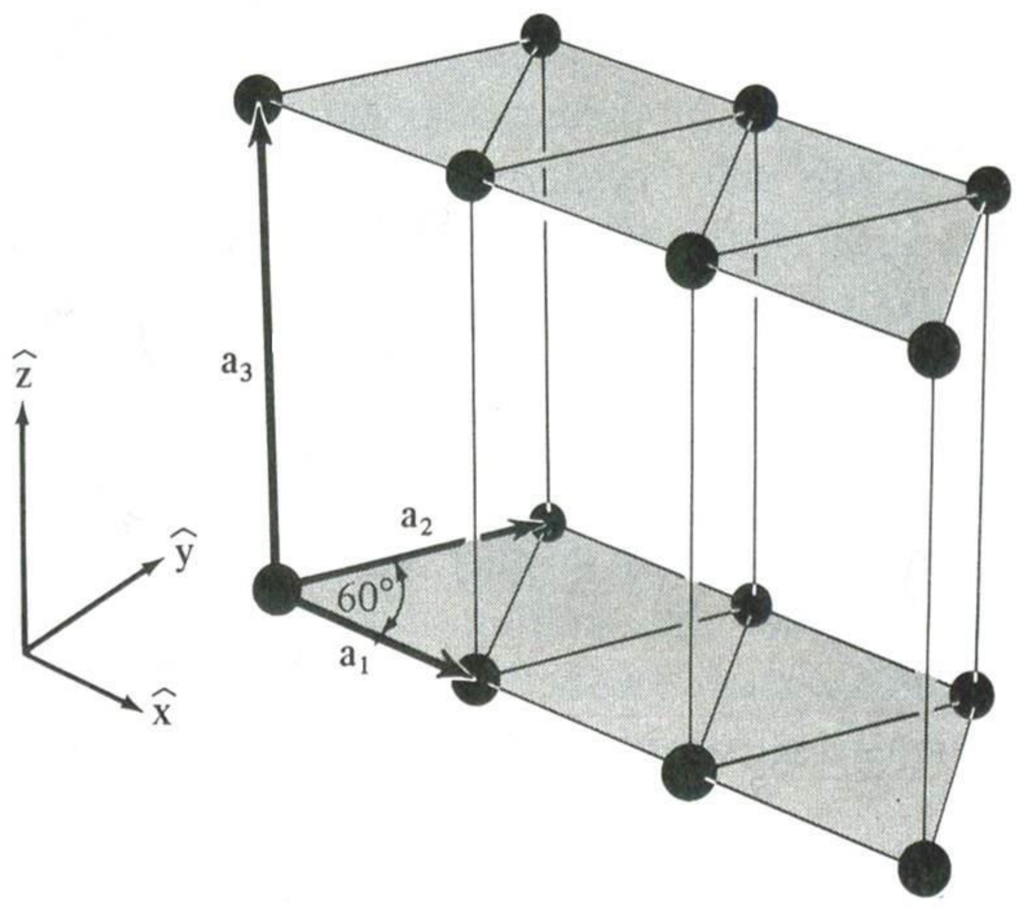
How many atoms do you have in the unit cell when you see it as a SC ?

How many atoms do you have in the unit cell when you see it as a FCC lattice ?



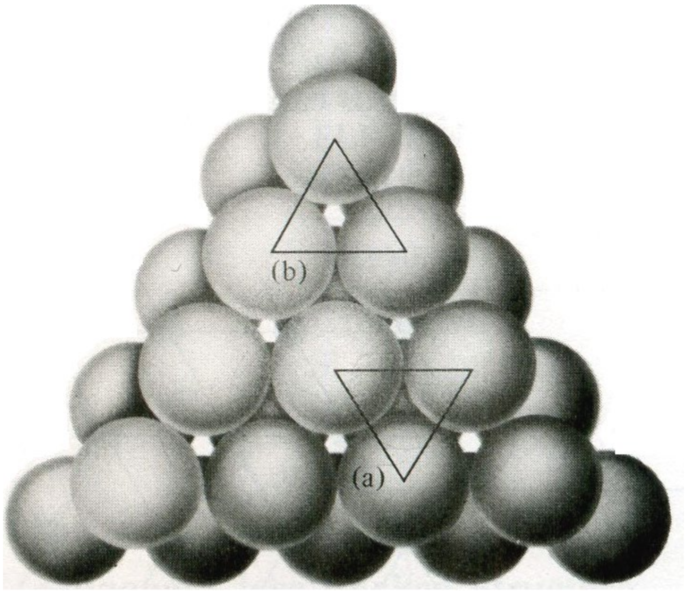
$$\begin{cases} \overrightarrow{a_1} = a\hat{x} \\ \overrightarrow{a_2} = a\hat{y} \\ \overrightarrow{a_3} = a\hat{z} \end{cases}$$

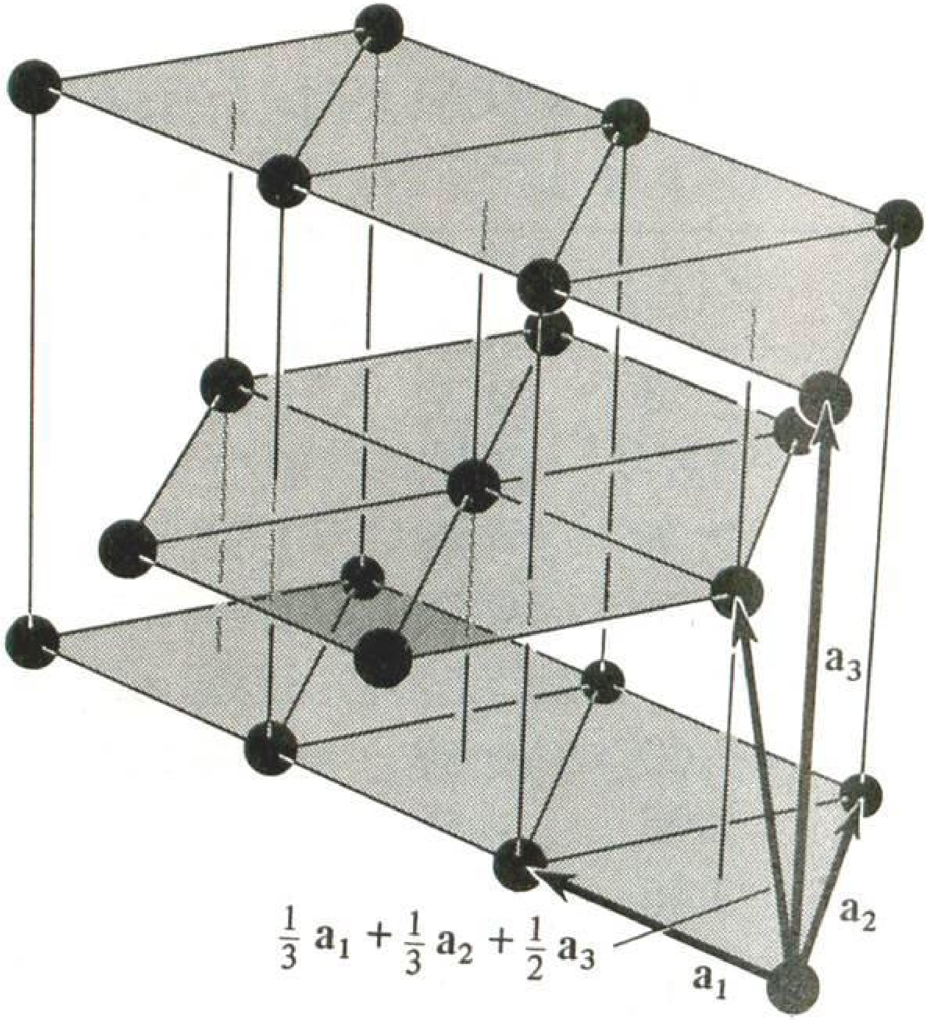
Simple Hexagonal Lattice



$$\begin{cases} \overrightarrow{a_1} = a\hat{x} \\ \overrightarrow{a_2} = a(\frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y}) \\ \overrightarrow{a_3} = c\hat{z} \end{cases}$$

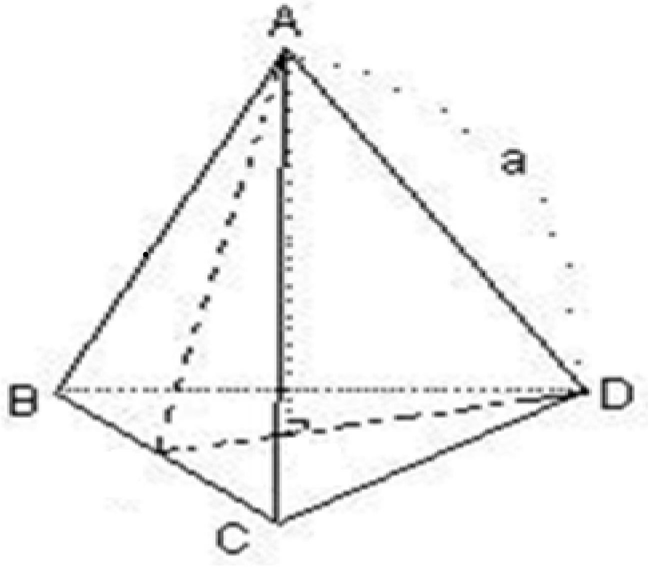
Hexagonal Close Pack (HCP)





Hexagonal Close Pack (HCP)

Regular tetrahedron



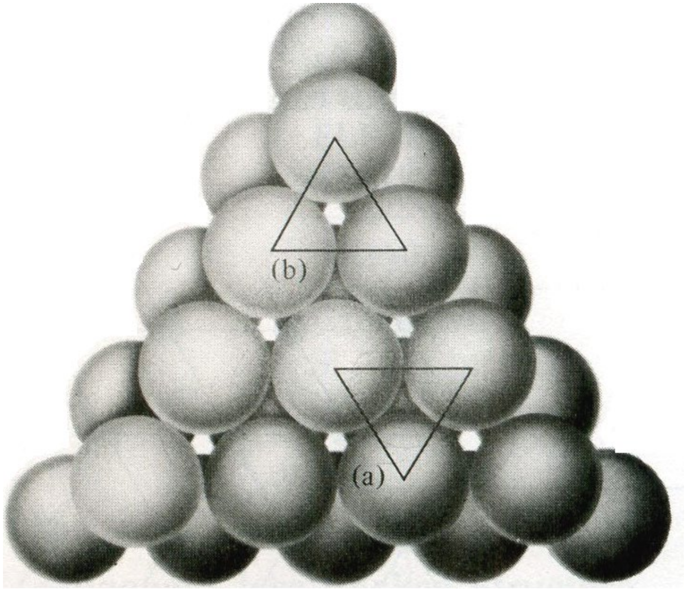
In high school mathematics class, you might have learned that the height of regular tetrahedron can be related to the length of edge.

$$h = a\sqrt{2/3}$$

Show that the 3rd lattice length, perpendicular the to plane lattice, is

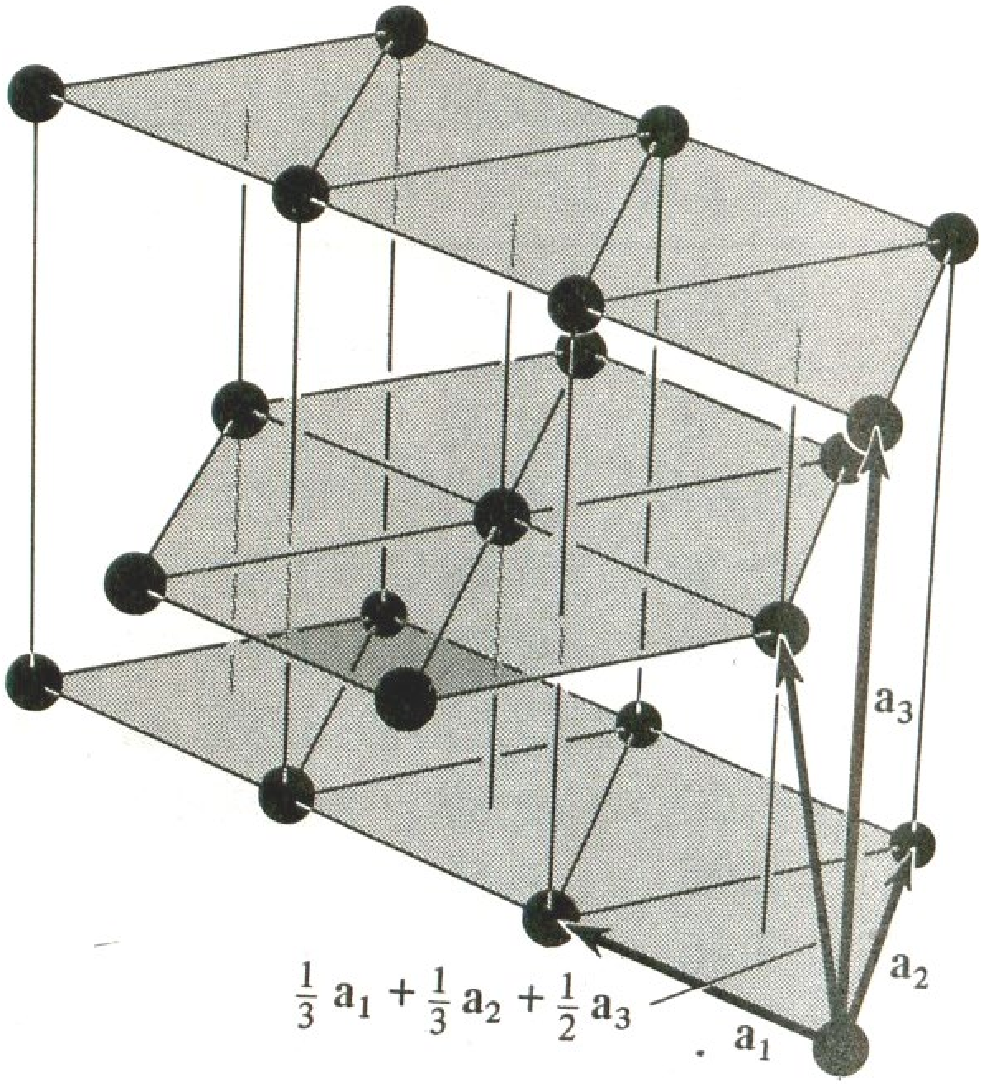
$$c = a\sqrt{8/3}$$

Hexagonal Close Pack (HCP)

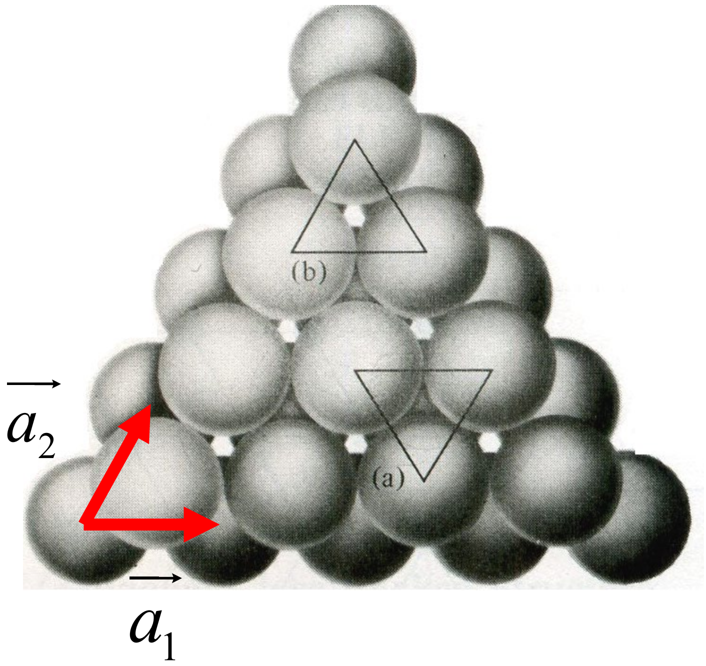


$$\overrightarrow{\tau_1} = 0$$

$$\overrightarrow{\tau_2} = \frac{1}{3}(\overrightarrow{a_1} + \overrightarrow{a_2}) + \frac{1}{2}\overrightarrow{a_3}$$



FCC and Close-Pack



$$\vec{\tau}_1 = 0$$

$$\vec{\tau}_2 = \frac{1}{3}(\vec{a}_1 + \vec{a}_2) + \frac{1}{3}\vec{a}_3$$

$$\vec{\tau}_3 = \vec{\tau}_2 + \frac{1}{3}(\vec{a}_1 + \vec{a}_2) + \frac{1}{3}\vec{a}_3 = 2\vec{\tau}_2$$

$$\vec{a}_1 = (a, 0, 0)$$

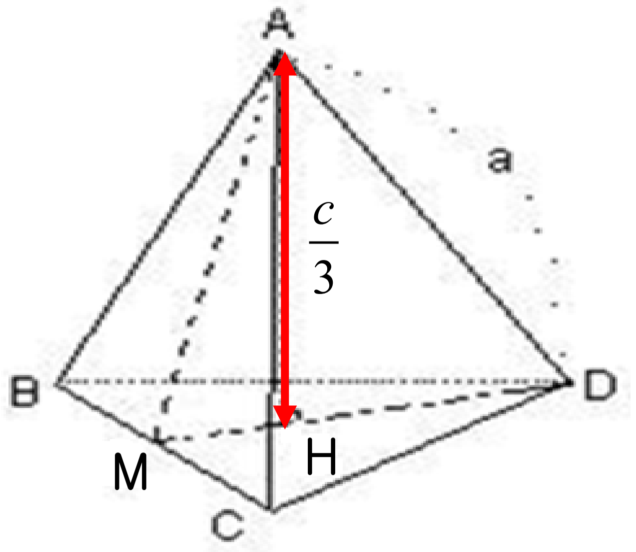
$$\vec{a}_2 = (\frac{a}{2}, \frac{\sqrt{3}a}{2}, 0)$$

$$\vec{a}_3 = (0, 0, c)$$

FCC is a type of closed-pack structure, when you look it at from the [111] axis direction

FCC and Close-Pack

FCC is a type of closed-pack structure, when you look it at from the [111] axis direction



$$c = \sqrt{6}a$$

$$\overline{DM} = \frac{\sqrt{3}}{2}a$$

$$\overline{DH} = \frac{2}{3}\overline{DM} = \frac{\sqrt{3}}{3}a$$

$$(\overline{AH})^2 = (\overline{AD})^2 - (\overline{DH})^2$$

$$(\overline{AH})^2 = a^2 - \frac{1}{3}a^2 = \frac{2}{3}a^2$$

$$\therefore \overline{AH} = \sqrt{\frac{2}{3}}a$$

Because FCC Structure has 3 layers,

$$c = 3\overline{AH}$$

$$c = \sqrt{6}a$$