

Simple Cubic lattice Lattice vectors

$1 \times 1 \times 1$ unit cell

$$\mathbf{V}_1 = a(1, 0, 0)$$

$$\mathbf{V}_2 = a(0, 1, 0)$$

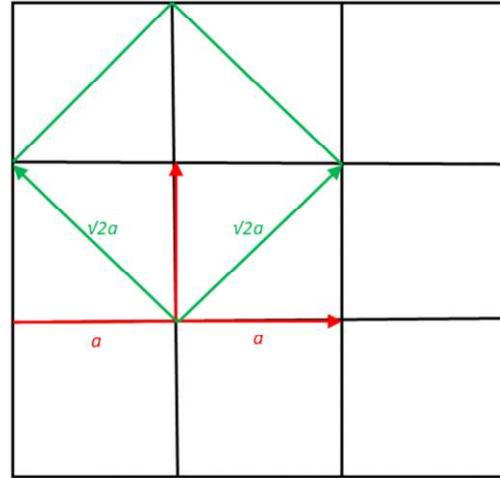
$$\mathbf{V}_3 = a(0, 0, 1)$$

$\sqrt{2} \times \sqrt{2} \times 1$ supercell

$$\mathbf{V}'_1 = a(1, 1, 0)$$

$$\mathbf{V}'_2 = a(-1, 1, 0)$$

$$\mathbf{V}'_3 = a(0, 0, 1)$$



Relation between the lattice vectors of
 $1 \times 1 \times 1$ unit cell and $\sqrt{2} \times \sqrt{2} \times 1$ supercell

$$\mathbf{V}'_1 = \mathbf{V}_1 + \mathbf{V}_2$$

$$\mathbf{V}'_2 = -\mathbf{V}_1 + \mathbf{V}_2$$

$$\mathbf{V}'_3 = \mathbf{V}_3$$

Transformation matrix (TRMAT)

$$\begin{vmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

Fig. 1: Relation between the lattice vectors of $1 \times 1 \times 1$ unit cell and $\sqrt{2} \times \sqrt{2} \times 1$ supercell and the corresponding transformation matrix of simple cubic lattice.

Hexagonal lattice Lattice vectors

$1 \times 1 \times 1$ unit cell

$$\mathbf{V}_1 = a(1, 0, 0)$$

$$\mathbf{V}_2 = a(-1/2, \sqrt{3}/2, 0)$$

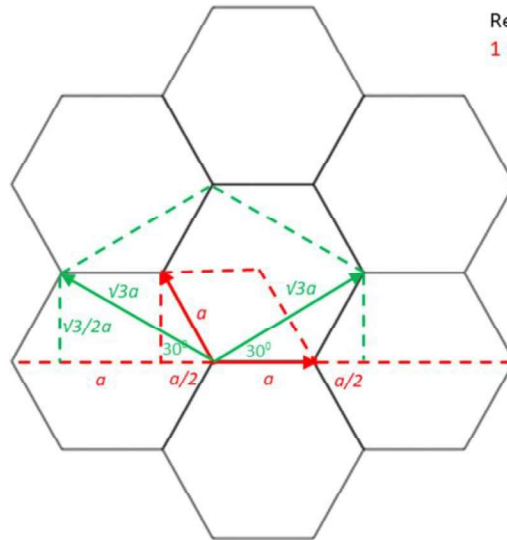
$$\mathbf{V}_3 = a(0, 0, c/a)$$

$\sqrt{3} \times \sqrt{3} \times 1$ supercell

$$\mathbf{V}'_1 = a(3/2, \sqrt{3}/2, 0)$$

$$\mathbf{V}'_2 = a(-3/2, \sqrt{3}/2, 0)$$

$$\mathbf{V}'_3 = a(0, 0, c/a)$$



Relation between the lattice vectors of
 $1 \times 1 \times 1$ unit cell and $\sqrt{3} \times \sqrt{3} \times 1$ supercell

$$\mathbf{V}'_1 = 2\mathbf{V}_1 + \mathbf{V}_2$$

$$\mathbf{V}'_2 = -\mathbf{V}_1 + \mathbf{V}_2$$

$$\mathbf{V}'_3 = \mathbf{V}_3$$

Transformation matrix (TRMAT)

$$\begin{vmatrix} 2 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

Fig. 2: Relation between the lattice vectors of $1 \times 1 \times 1$ unit cell and $\sqrt{3} \times \sqrt{3} \times 1$ supercell and the corresponding transformation matrix of hexagonal lattice.