

Rede de Bravais ou rede cristalina

Uma rede de Bravais é um conjunto infinito de pontos definido por uma combinação linear de vetores primitivos linearmente independentes:

$$\mathbf{R}_n = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 = \sum_{i=1}^d n_i \mathbf{a}_i, n_i \in \mathbb{Z} \quad n(\mathbf{r}) = \sum_{\mathbf{R}_1} \delta(\mathbf{r} - \mathbf{R}_1)$$

› A soma de dois vetores de da rede pertence à rede:

$$\mathbf{T} = \mathbf{R}_n - \mathbf{R}_{n'} \text{ Vetor de translação}$$

› A vizinhança de todos os pontos da rede é a mesma.

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$$n(\mathbf{r}) = \sum_1 \delta(\mathbf{r} - \mathbf{R}_1)$$

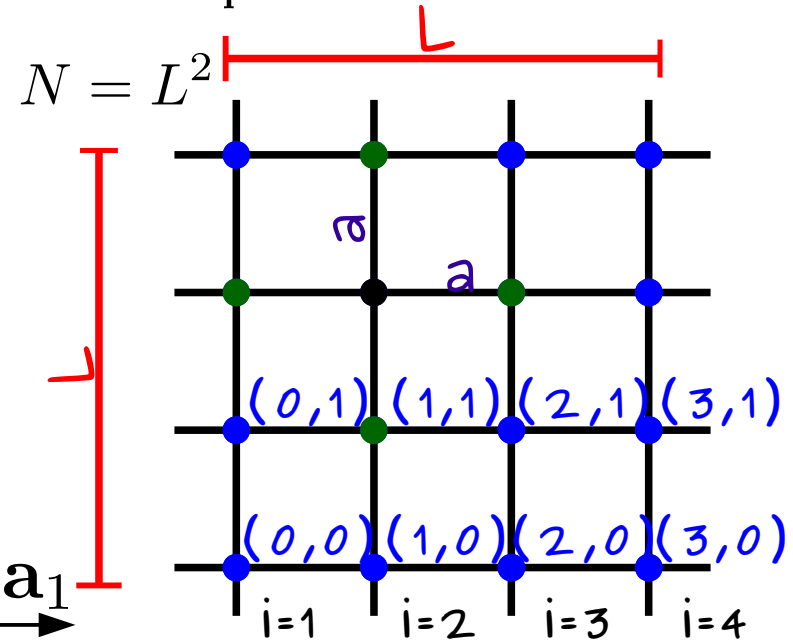
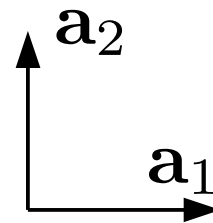
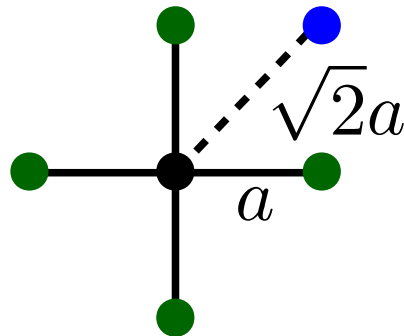
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Número de coordenação
ou número de primeiros
vizinhos: rede quadrada

$$z = 4$$



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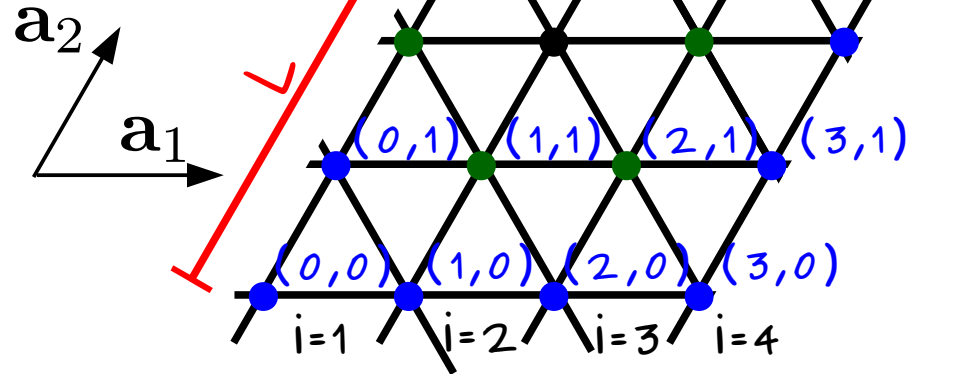
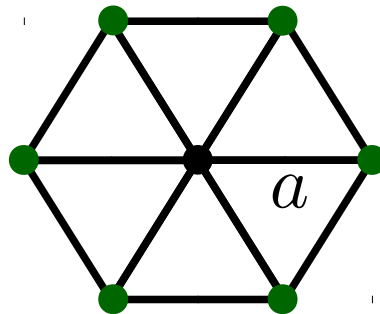
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Número de coordenação
ou número de primeiros
vizinhos: rede triangular

$$z = 6$$

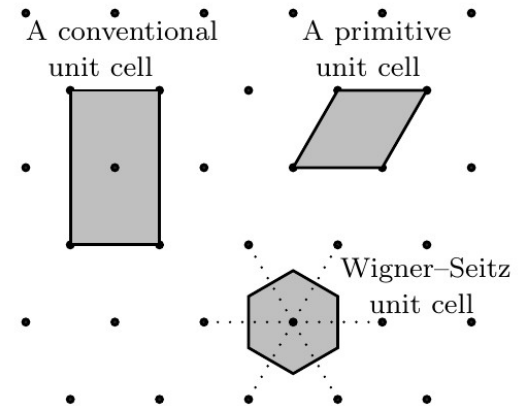


Célula unitária – rede com uma base

Uma célula unitária é o bloco fundamental de uma rede de Bravais (não é única).

- Uma célula unitária primitiva contém exatamente um ponto da rede;
- Dado um ponto da rede de Bravais, a região do espaço mais próximos dele do que de qualquer outro ponto define a célula de Wigner-Seitz.

Em cada célula unitária, a localização dos componentes é dada pelos *vetores de base*



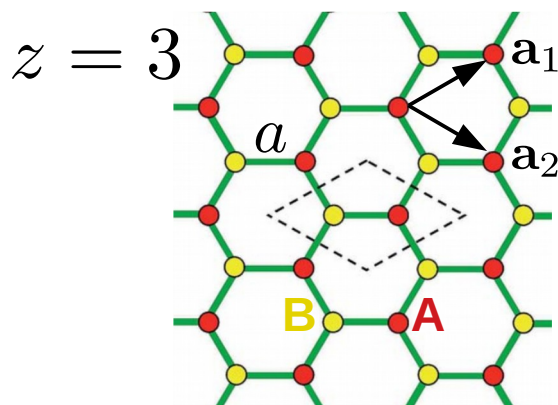
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Rede favo de mel ou colmeia. $N = 2L^2$

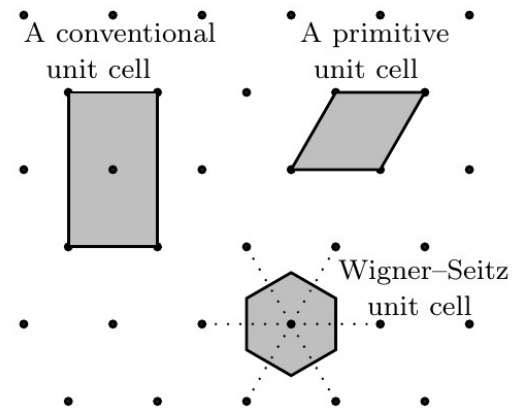


$$\mathbf{a}_1 = \frac{a}{2} (3\mathbf{i} + \sqrt{3}\mathbf{j}) \quad \mathbf{a}_2 = \frac{a}{2} (3\mathbf{i} - \sqrt{3}\mathbf{j})$$

$$\mathbf{R}_{n,A} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2$$

$$\mathbf{R}_{n,B} = \mathbf{R}_{n,A} - a\mathbf{i} = (n_1 - 1/3) \mathbf{a}_1 + (n_2 - 1/3) \mathbf{a}_2$$

$$n(\mathbf{r}) = \sum_{\mathbf{l}, \alpha} m_\alpha \delta(\mathbf{r} - \mathbf{R}_{\mathbf{l}} - \mathbf{x}_\alpha)$$



Simetrias – rede triangular

- 1) Simetria de rotação de 30° para qualquer ponto

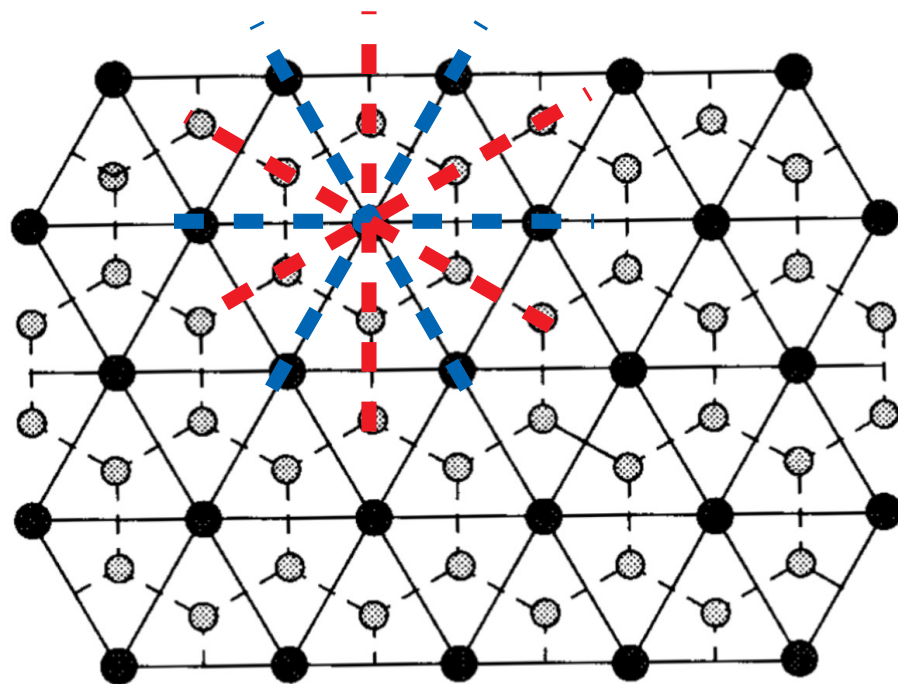
$$2\pi p/6, p = 0, \dots, 5$$

- 2) Simetria de reflexão: 6 linhas ligando 1^{os} e 2^{os} vizinhos.

- 3) Rede dual: rede favo de mel

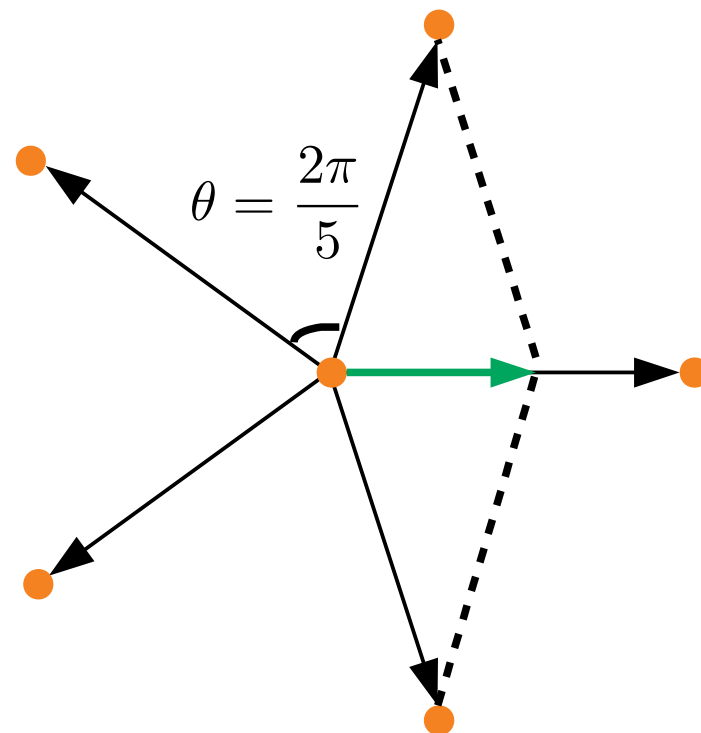
➤ Sítios no centro da plaqueta elementar.

- 4) Maior simetria rotacional em 2D



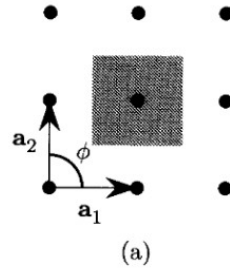
Pentágonos regulares proibidos

- De nossa definição original, sabemos que a soma de dois vetores de rede, tem que cair na rede;
- Rotações com $n=5$, 72° , proibidas!
- Não conseguimos preencher o plano com pentágonos regulares;
- Apenas $n=2,3,4$ e 6 permitidos.

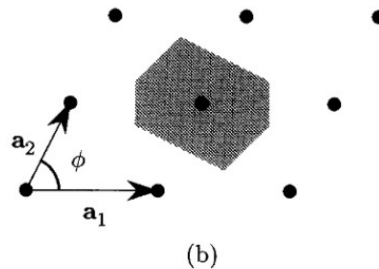


Redes de Bravais em 2D

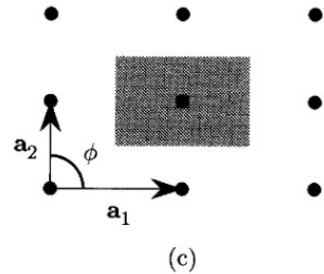
$n=4$, quadrada



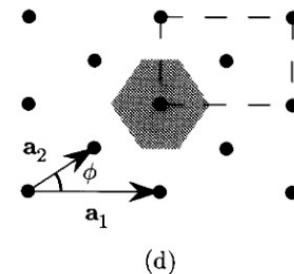
$n=2$, oblua



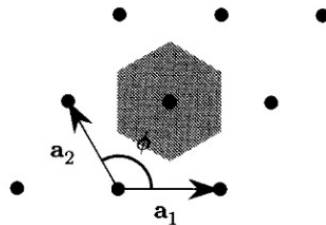
$n=2$, retangular



$n=2$, retangular centrada

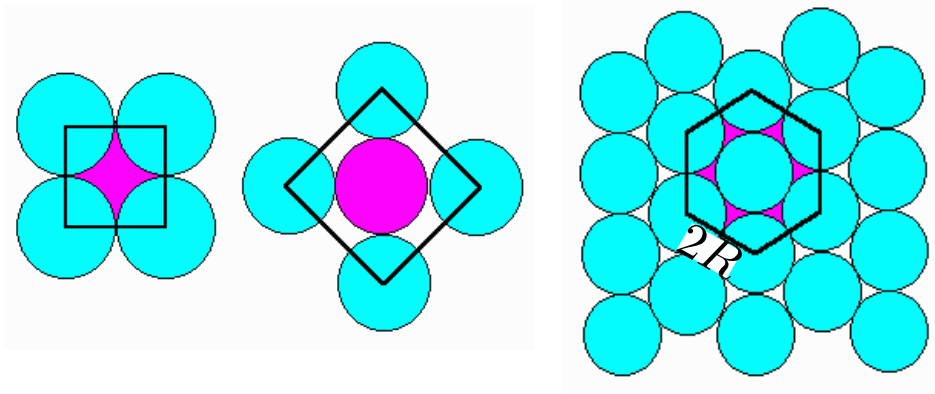


$n=6$, triangular



Empacotamento

- A rede triangular possui o melhor empacotamento de círculos em 2D;
- Situação energeticamente mais favorável pois “aproxima” os constituintes. Menos vazio.



$$A_{\circ} = \frac{3\sqrt{3}}{2} (2R)^2 = 6\sqrt{3}R^2$$

$$A_{\circ} = \left(1 + 6 \times \frac{1}{3}\right) \pi R^2 = 3\pi R^2$$

$$\frac{A_{\circ}}{A_{\circ}} = \frac{\pi\sqrt{3}}{6} = 0.907$$

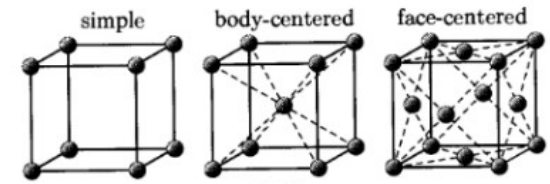
Redes de Bravais em 3D

Há 14 tipos de redes de Bravais:

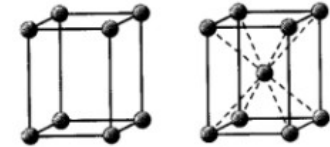
| System | Number of lattices in system | Lattice symbols | Restrictions on conventional cell axes and angles |
|--------------|------------------------------|---------------------------------|---|
| Triclinic | 1 | P | $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$ |
| Monoclinic | 2 | P,C | $a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta$ |
| Orthorhombic | 4 | P,C,I,F | $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$ |
| Tetragonal | 2 | P,I | $a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$ |
| Cubic | 3 | P or SC I or BCC F of FCC | $a = b = c$ $\alpha = \beta = \gamma = 90^\circ$ |
| Trigonal | 1 | R | $a = b = c$ $\alpha = \beta = \gamma < 120^\circ, \neq 90^\circ$ |
| Hexagonal | 1 | P | $a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$ |

$$\mathbf{R}_n = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$$

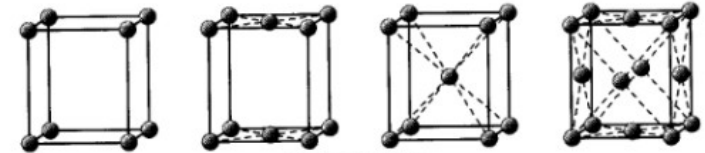
$$\mathbf{R}_n = [n_1 n_2 n_3]$$



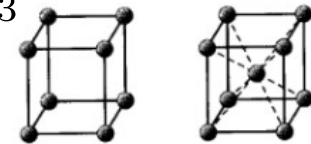
Cubic



Tetragonal



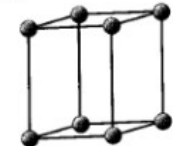
Orthorhombic



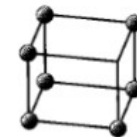
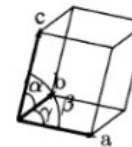
Monoclinic



Trigonal

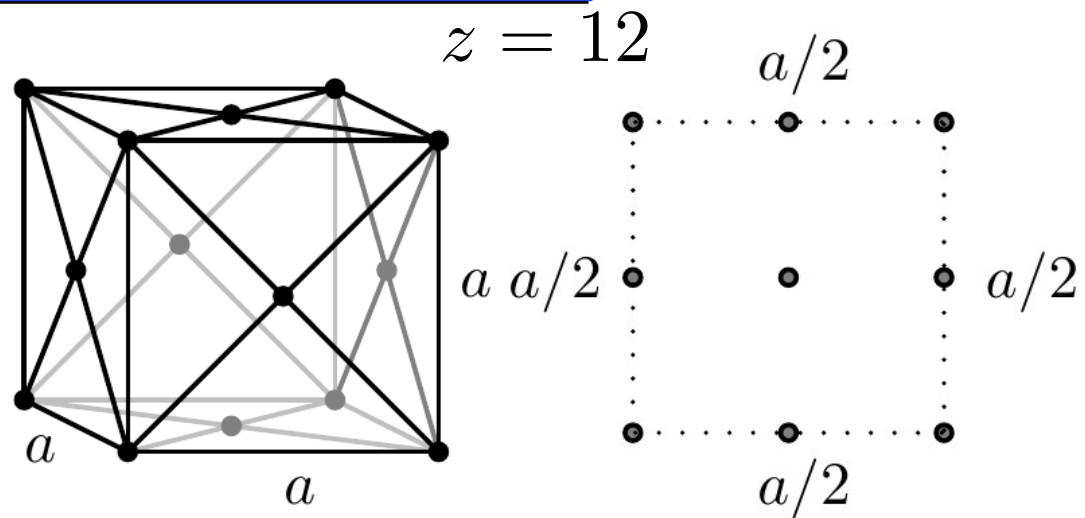
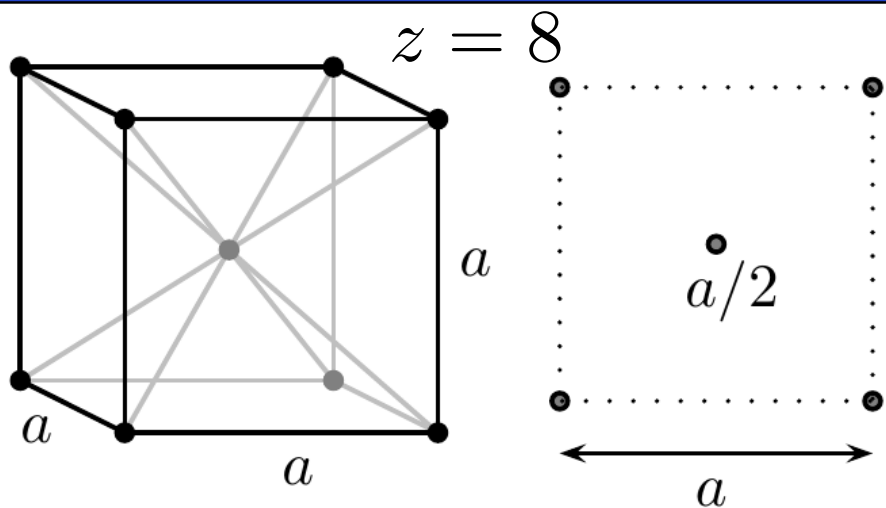


Trigonal and hexagonal



Triclinic

BCC e FCC



$$\mathbf{a}_1 = \frac{a}{2} [\bar{1}11] \quad \mathbf{a}_2 = \frac{a}{2} [1\bar{1}1] \quad \mathbf{a}_3 = \frac{a}{2} [11\bar{1}] \quad \mathbf{a}_1 = \frac{a}{2} [011] \quad \mathbf{a}_2 = \frac{a}{2} [101] \quad \mathbf{a}_3 = \frac{a}{2} [110]$$


$$\mathbf{R}_{n,A} = n_1 \mathbf{i} + n_2 \mathbf{j} + n_3 \mathbf{k} \quad \mathbf{R}_{n,B} = \mathbf{R}_{n,A} + \frac{a}{2} (\mathbf{i} + \mathbf{j} + \mathbf{k}) \quad \mathbf{R}_{n,A} = n_1 \mathbf{i} + n_2 \mathbf{j} + n_3 \mathbf{k} \quad \mathbf{R}_{n,B} = \mathbf{R}_{n,A} + \frac{a}{2} (\mathbf{i} + \mathbf{j})$$

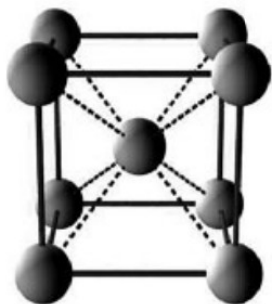
$$\mathbf{R}_{n,C} = \mathbf{R}_{n,A} + \frac{a}{2} (\mathbf{j} + \mathbf{k}) \quad \mathbf{R}_{n,D} = \mathbf{R}_{n,A} + \frac{a}{2} (\mathbf{i} + \mathbf{k})$$

Exemplos egrégios

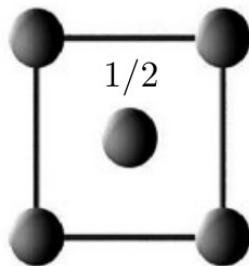
Sodium (Na)

Lattice = Cubic-I (bcc)

Basis = Na at [000] 




Plan view
unlabeled points at $z = 0, 1$

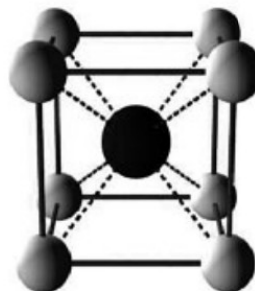


Caesium chloride (CsCl)

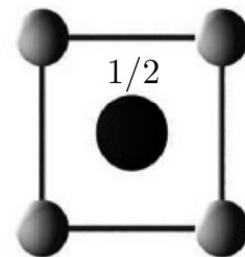
Lattice = Cubic-P

Basis = Cs at [000] 

and Cl at $[\frac{1}{2}\frac{1}{2}\frac{1}{2}]$ 




Plan view
unlabeled points at $z = 0, 1$

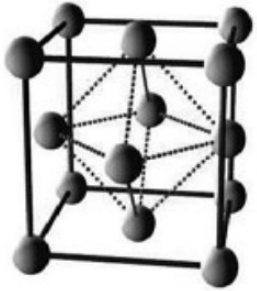


Exemplos egrégios

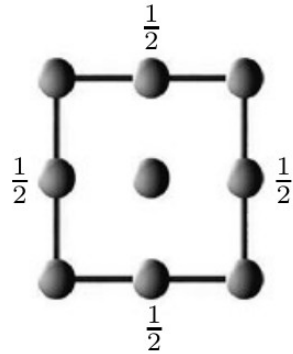
Copper(Cu)

Lattice = Cubic-F (fcc)

Basis = Cu at $[000]$ 




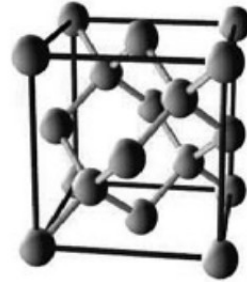
Plan view
unlabeled points at $z = 0, 1$



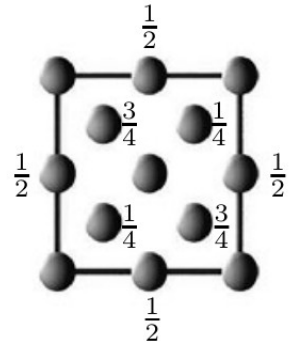
Diamond (C); also Si and Ge

Lattice = Cubic-F (fcc)

Basis = C at $[000]$ 
and C at $[\frac{1}{4}\frac{1}{4}\frac{1}{4}]$




Plan view
unlabeled points at $z = 0, 1$




Exemplos egrégios

Sodium Chloride (NaCl)

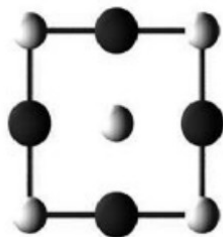
Lattice = Cubic-F (fcc)

Basis = Na at $[000]$ 

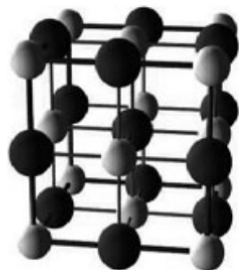
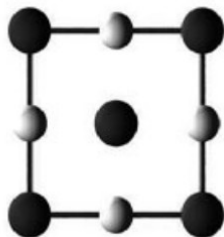
and Cl at $[\frac{1}{2}\frac{1}{2}\frac{1}{2}]$ 

Plan view

$z = 0, 1$ layer



$z = \frac{1}{2}$ layer



$\text{BaTi}_{1/2}\text{Mn}_{1/2}\text{O}_3$

