bcc Lattice and Primitive Unit Cell

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1 bcc Lattice (beware of tensors)

The body-centered cubic (BCC) lattice is defined by a conventional cubic unit cell with lattice constant a. The basis vectors of the conventional unit cell in Cartesian coordinates are:

$$\mathbf{a}_1 = a(1,0,0), \quad \mathbf{a}_2 = a(0,1,0), \quad \mathbf{a}_3 = a(0,0,1) \tag{1}$$

In tensor notation, these vectors are contravariant, expressed as $\mathbf{a}_i = a_i^\mu \mathbf{e}_\mu$, where $\mathbf{e}_\mu$ ($\mu = 1,2,3$) are the Cartesian basis vectors, and:

$$a_i^\mu = a\delta_i^\mu \tag{2}$$

where δ_i^μ is the Kronecker delta ($\delta_i^\mu = 1$ if $i = \mu$, else 0).
The BCC crystal structure has a basis of two atoms per conventional unit cell, located at:

$$\mathbf{r}_1 = (0,0,0), \quad \mathbf{r}_2 = \frac{a}{2}(1,1,1) \tag{3}$$

In tensor form:

$$r_1^\mu = (0,0,0), \quad r_2^\mu = \frac{a}{2}(1,1,1) \tag{4}$$

The position of any atom in the crystal is:

$$\mathbf{R} = n^i \mathbf{a}_i + \mathbf{r}_j, \quad R^\mu = n^i a_i^\mu + r_j^\mu \tag{5}$$

where $n^i \in \mathbb{Z}$ and $j = 1,2$. Substituting:

$$R^\mu = n^i a\delta_i^\mu + r_j^\mu = a(n^1\delta_1^\mu + n^2\delta_2^\mu + n^3\delta_3^\mu) + r_j^\mu \tag{6}$$

For $j = 1$:

$$R^\mu = a(n^1, n^2, n^3) \tag{7}$$

For $j = 2$:

$$R^\mu = a\left(n^1 + \frac{1}{2}, n^2 + \frac{1}{2}, n^3 + \frac{1}{2}\right) \tag{8}$$

This generates all BCC lattice positions.

2 Metric Tensor and Volume of Conventional Unit Cell

The metric tensor is:

$$g_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j = a_i^\mu a_j^\nu \delta_{\mu\nu} \tag{9}$$

Since $\mathbf{a}_i$ are orthogonal:

$$g_{ij} = a^2 \delta_{ij} \tag{10}$$

The volume is given by the scalar triple product:

$$V = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)| = |\varepsilon^{\mu\nu\lambda} a_{1\mu} a_{2\nu} a_{3\lambda}| \tag{11}$$

Substituting:

$$V = \varepsilon^{\mu\nu\lambda} (a\delta_{1\mu})(a\delta_{2\nu})(a\delta_{3\lambda}) = a^3 \varepsilon^{123} = a^3 \tag{12}$$

The volume is $V = a^3$.

3 Primitive Unit Cell

The primitive unit cell contains one lattice point. Suitable primitive vectors are:

$$\mathbf{b}_1 = \frac{a}{2}(1,1,-1), \quad \mathbf{b}_2 = \frac{a}{2}(-1,1,1), \quad \mathbf{b}_3 = \frac{a}{2}(1,-1,1) \tag{13}$$

In tensor notation:

$$b_i^\mu = \frac{a}{2} \begin{cases} (1,1,-1) & i = 1 \\ (-1,1,1) & i = 2 \\ (1,-1,1) & i = 3 \end{cases} \tag{14}$$

Lattice points are generated by:

$$R^\mu = m^i b_i^\mu, \quad m^i \in \mathbb{Z} \tag{15}$$

4 Metric Tensor for Primitive Unit Cell

The metric tensor is:

$$g_{ij} = \mathbf{b}_i \cdot \mathbf{b}_j = b_i^\mu b_j^\nu \delta_{\mu\nu} \tag{16}$$

Computing:

$$g_{11} = \frac{a^2}{4}(1^2 + 1^2 + (-1)^2) = \frac{3a^2}{4} \tag{17}$$

$$g_{12} = \frac{a^2}{4}[(1)(-1) + (1)(1) + (-1)(1)] = -\frac{a^2}{4} \tag{18}$$

$$g_{13} = \frac{a^2}{4}[(1)(1) + (1)(-1) + (-1)(1)] = -\frac{a^2}{4} \tag{19}$$

$$g_{22} = \frac{a^2}{4}[(-1)^2 + 1^2 + 1^2] = \frac{3a^2}{4} \tag{20}$$

$$g_{23} = \frac{a^2}{4}[(-1)(1) + (1)(-1) + (1)(1)] = -\frac{a^2}{4} \tag{21}$$

$$g_{33} = \frac{a^2}{4}[1^2 + (-1)^2 + 1^2] = \frac{3a^2}{4} \tag{22}$$

Thus:

$$g_{ij} = \frac{a^2}{4}\begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix} \tag{23}$$

5 Volume of Primitive Unit Cell

The volume is:

$$V = |\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3)| = |\varepsilon^{\mu\nu\lambda} b_{1\mu} b_{2\nu} b_{3\lambda}| \tag{24}$$

Compute:

$$\mathbf{b}_2 \times \mathbf{b}_3 = \frac{a^2}{4}\begin{vmatrix} \hat{\mathbf{e}}_1 & \hat{\mathbf{e}}_2 & \hat{\mathbf{e}}_3 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix} = \frac{a^2}{4}[2\hat{\mathbf{e}}_1 + 2\hat{\mathbf{e}}_2 + 0\hat{\mathbf{e}}_3] = \frac{a^2}{2}(1,1,0) \tag{25}$$

$$V = \left|\frac{a}{2}(1,1,-1) \cdot \frac{a^2}{2}(1,1,0)\right| = \frac{a^3}{4}|1 \cdot 1 + 1 \cdot 1 + (-1) \cdot 0| = \frac{a^3}{4} \cdot 2 = \frac{a^3}{2} \tag{26}$$

The volume is $\frac{a^3}{2}$, half the conventional cell volume, confirming one lattice point.

6 Basis in Primitive Unit Cell

The primitive unit cell has one lattice point with a basis of one atom at:

$$r^\mu = (0,0,0) \tag{27}$$

Positions are:

$$R^\mu = m^i b_i^\mu \tag{28}$$

7 Transformation Between Conventional and Primitive Cells

Express primitive vectors as:

$$\mathbf{b}_1 = \frac{1}{2}(\mathbf{a}_1 + \mathbf{a}_2 - \mathbf{a}_3) \tag{29}$$

$$\mathbf{b}_2 = \frac{1}{2}(-\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3) \tag{30}$$

$$\mathbf{b}_3 = \frac{1}{2}(\mathbf{a}_1 - \mathbf{a}_2 + \mathbf{a}_3) \tag{31}$$

In tensor form:

$$b_i^\mu = T_i^{\ j} a_j^\mu, \quad T_i^{\ j} = \frac{1}{2}\begin{pmatrix} 1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{pmatrix} \tag{32}$$

The volume ratio is:

$$\det(T) = \frac{1}{8}\begin{vmatrix} 1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix} = \frac{1}{8}[1(1\cdot 1 - 1\cdot(-1)) - 1((-1)\cdot 1 - 1\cdot 1) + (-1)((-1)\cdot(-1) - 1\cdot 1)] = \frac{1}{2} \tag{33}$$

Thus:

$$V_{\text{primitive}} = |\det(T)| V_{\text{conventional}} = \frac{1}{2}\cdot a^3 = \frac{a^3}{2} \tag{34}$$

8 Conclusion

The BCC lattice is described by:

- **Conventional unit cell**: Basis vectors $a_i^\mu = a\delta_i^\mu$, two-atom basis at $r_1^\mu = (0,0,0)$, $r_2^\mu = \frac{a}{2}(1,1,1)$. Volume a^3, metric tensor $g_{ij} = a^2\delta_{ij}$.
- **Primitive unit cell**: Basis vectors $b_1^\mu = \frac{a}{2}(1,1,-1)$, $b_2^\mu = \frac{a}{2}(-1,1,1)$, $b_3^\mu = \frac{a}{2}(1,-1,1)$, single-atom basis at $r^\mu = (0,0,0)$. Volume $\frac{a^3}{2}$, metric tensor $g_{ij} = \frac{a^2}{4}\begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix}$.

The transformation $T_i^{\ j}$ and volume calculations prove the primitive cell contains one lattice point, consistent with the BCC structure.