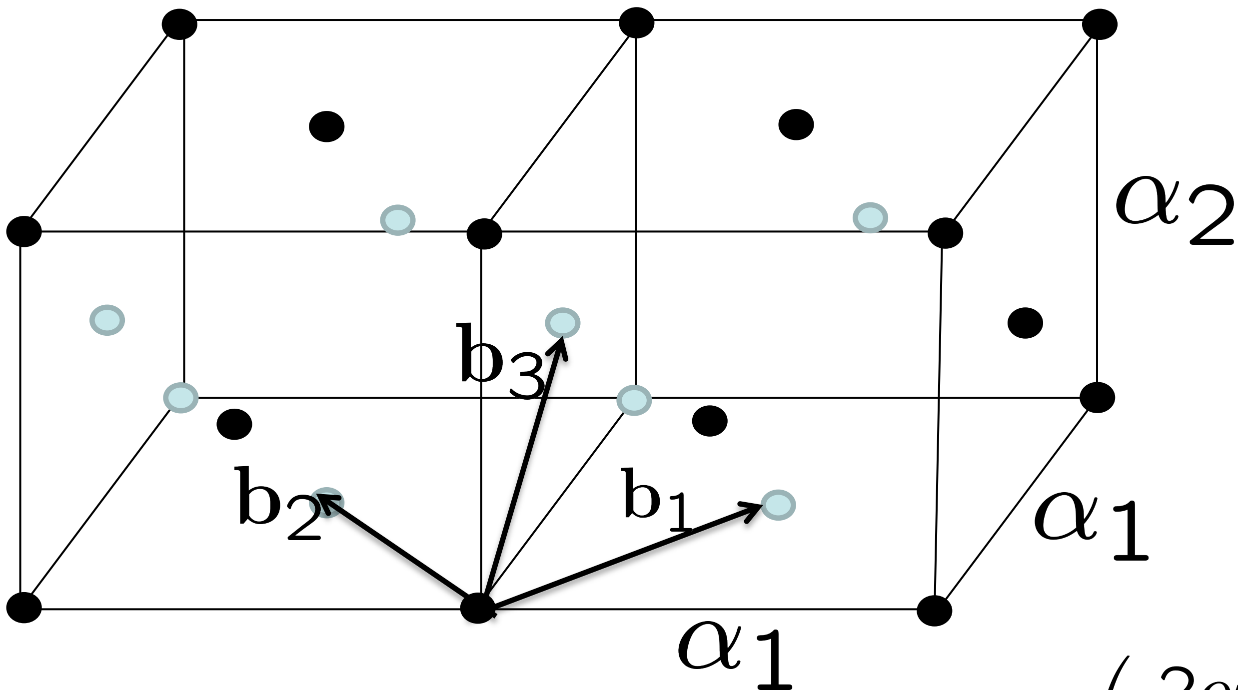
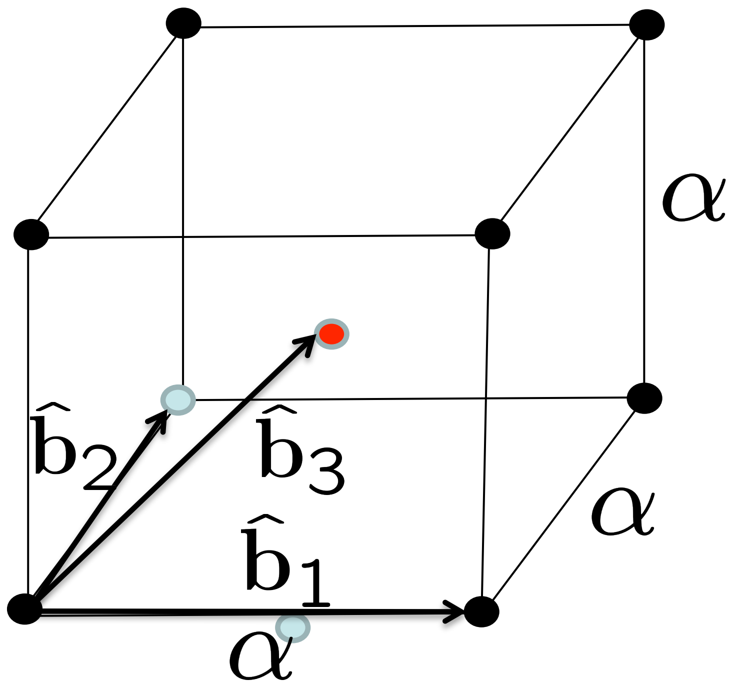
2. Face-centred tetragonal (fct)



$$\mathbf{B}^T\mathbf{B} = \frac{1}{4}\begin{pmatrix} 2\alpha_1^2 & 0 & \alpha_1^2 \\ 0 & 2\alpha_1^2 & \alpha_1^2 \\ \alpha_1^2 & \alpha_1^2 & \alpha_1^2 + \alpha_2^2 \end{pmatrix}$$

3. Body-centred cubic (bcc)



Could take the basis vectors as $\hat{\mathbf{b}}_i$ shown, but the conventional and more symmetric choice is

$$\mathbf{B} = \frac{\alpha}{2}\mathbf{Q}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}, \; \mathbf{Q} \in O(3)$$

for which

$$\mathbf{B}^T\mathbf{B} = \frac{\alpha^2}{4}\begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix}.$$

Body-centered tetragonal (bct) treated similarly.

$GL(3,\mathbb{Z}) = \{\boldsymbol{\mu} = (\mu_{ij}) : \mu_{ij} \in \mathbb{Z}, \det \boldsymbol{\mu} = \pm 1\}.$

Theorem $\mathcal{L}(\mathbf{B}) = \mathcal{L}(\mathbf{C})$ iff

$$\mathbf{B} = \mathbf{C}\boldsymbol{\mu}, \text{ for some } \boldsymbol{\mu} \in GL(3,\mathbb{Z}).$$

Proof. Let $\mathbf{B} = (\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3)$, $\mathbf{C} = (\mathbf{c}_1, \mathbf{c}_2, \mathbf{c}_3)$.

If $\mathcal{L}(\mathbf{B}) = \mathcal{L}(\mathbf{C})$ then $\mathbf{b}_i = \mu_{ji}\mathbf{c}_j$ for some $\boldsymbol{\mu} = (\mu_{ij}) \in \mathbb{Z}^{3\times 3}$, so that $\mathbf{B} = \mathbf{C}\boldsymbol{\mu}$. Similarly $\mathbf{C} = \mathbf{B}\boldsymbol{\mu}'$ for some $\boldsymbol{\mu}' \in \mathbb{Z}^{3\times 3}$. So $\boldsymbol{\mu}' = \boldsymbol{\mu}^{-1}$ and $\boldsymbol{\mu} \in GL(3,\mathbb{Z})$.

Conversely, if $\mathbf{B} = \mathbf{C}\boldsymbol{\mu}$ then $\mathbf{b}_i = \mu_{ji}\mathbf{c}_j$ and so $\mathcal{L}(\mathbf{B}) \subset \mathcal{L}(\mathbf{C})$. Similarly $\mathcal{L}(\mathbf{C}) \subset \mathcal{L}(\mathbf{B})$. $\square$

Corollary. If $\mathbf{F} \in GL(3, \mathbb{R})$, then $\mathcal{L}(\mathbf{FB}) = \mathcal{L}(\mathbf{B})$ iff

$$\mathbf{F} = \mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1} \text{ for some } \boldsymbol{\mu} \in GL(3, \mathbb{Z}).$$

Definition. The *point group* $P(\mathbf{B})$ of $\mathcal{L}(\mathbf{B})$ is the set of $\mathbf{Q} \in O(3)$ such that $\mathcal{L}(\mathbf{QB}) = \mathcal{L}(\mathbf{B})$.

By the Corollary,

$$P(\mathbf{B}) = \{\mathbf{Q} \in O(3) : \mathbf{B}^{-1}\mathbf{QB} \in GL(3, \mathbb{Z})\}.$$

If $\mathbf{B}^{-1}\mathbf{QB} = \boldsymbol{\mu} \in GL(3, \mathbb{Z})$ then $\boldsymbol{\mu}^T\boldsymbol{\mu} = \mathbf{B}^T\mathbf{B}^{-T}$, and so $P(\mathbf{B})$ is a *finite* group.

If $\mathbf{R} \in O(3)$ then

$$\begin{aligned} P(\mathbf{RB}) &= \{\mathbf{Q} : \mathbf{R}^T\mathbf{QR} \in \mathcal{L}(\mathbf{B})\} \\ &= \{\mathbf{R}\tilde{\mathbf{Q}}\mathbf{R}^T : \tilde{\mathbf{Q}} \in \mathcal{L}(\mathbf{B})\} \\ &= \mathbf{R}P(\mathbf{B})\mathbf{R}^T, \end{aligned}$$

so that $P(\mathbf{RB})$ is orthogonally conjugate to $P(\mathbf{B})$.

The point groups of the simple cubic ($\mathbf{B} = \alpha\mathbf{Q1}$), fcc and bcc lattices are the same, namely (taking $\mathbf{Q} = \mathbf{1}$) the cubic group P^c consisting of the 48 orthogonal tranformations mapping the unit cube $(0,1)^3$ into itself.

Thus the point group does not discriminate between the different possible cubic lattices, and to do this one needs to consider the *lattice group*

$$L(\mathbf{B}) = \{\boldsymbol{\mu} \in GL(3,\mathbb{Z}) : \mathbf{B}\boldsymbol{\mu}\mathbf{B}^{-1} \in O(3)\}$$

$L(\mathbf{QB}) = L(\mathbf{B})$ for all $\mathbf{Q} \in O(3)$. However $L(\mathbf{B})$ depends on the lattice basis, so that

$$L(\mathbf{B}\boldsymbol{\mu}) = \boldsymbol{\mu}^{-1}L(\mathbf{B})\boldsymbol{\mu} \text{ for all } \boldsymbol{\mu} \in GL(3,\mathbb{Z}).$$

The corresponding conjugacy classes determine 14 distinct Bravais lattices (triclinic, monoclinic, orthorhombic, rhombohedral, tetragonal, hexagonal and cubic).

We now fix a reference lattice $\mathcal{L}(\mathbf{B})$ with $\mathbf{B} \in GL^+(3, \mathbb{R})$, and suppose that there is a free-energy function $\varphi(\mathbf{C}, \theta)$ defined for $\mathbf{C}$ in an open neighbourhood D of $\mathbf{B}$ in $GL^+(3, \mathbb{R})$ satisfying

$$\mathbf{Q}D\boldsymbol{\mu} \subset D \text{ for all } \mathbf{Q} \in SO(3), \boldsymbol{\mu} \in GL^+(3, \mathbb{Z})(= SL(3, \mathbb{Z}))$$

and temperatures θ in some interval I, such that for all $\mathbf{C} \in D, \theta \in I$

(i) $\varphi(\mathbf{QC}, \theta) = \varphi(\mathbf{C}, \theta)$ for all $\mathbf{Q} \in SO(3)$,

(ii) $\varphi(\mathbf{C}\boldsymbol{\mu}, \theta) = \varphi(\mathbf{C}, \theta)$ for all $\boldsymbol{\mu} \in GL^+(3, \mathbb{Z})$.

That is, the free-energy is rotationally invariant and depends only on the lattice $\mathcal{L}(\mathbf{C})$.

We now use the Cauchy-Born rule (an implicit coarse-graining) to relate the macroscopic free-energy density ψ to φ. Choosing a reference configuration in which the crystal lattice is $\mathbf{B}$, we assume that

$$\psi(\mathbf{A},\theta) = \varphi(\mathbf{AB},\theta), \text{ for } \mathbf{A} \in D(\psi), \theta \in I,$$

where $D(\psi) = D\mathbf{B}^{-1}$.

Thus ψ inherits the invariances for all $\mathbf{A} \in D(\psi), \theta \in I$,
(i) $\psi(\mathbf{QA},\theta) = \psi(\mathbf{A},\theta)$ for all $\mathbf{Q} \in SO(3)$,
(ii) $\psi(\mathbf{AB}\boldsymbol{\mu}\mathbf{B}^{-1},\theta) = \psi(\mathbf{A},\theta)$ for all $\boldsymbol{\mu} \in GL^+(3,\mathbb{Z})$.

Hence ψ has symmetry group $\mathcal{S} = \mathbf{B}\,GL^+(3,\mathbb{Z})\,\mathbf{B}^{-1}$, which is a subgroup of $SL(3,\mathbb{R})$.

Martensitic phase transformations

We now assume that $\varphi(\cdot,\theta)$ is bounded below for each $\theta \in I$ and attains a minimum. We can suppose that the minimum value is zero. Hence also the minimum value of $\psi(\cdot,\theta)$ is zero.

$$\text{Let } K(\theta) = \{\mathbf{A} \in D(\psi) : \psi(\mathbf{A},\theta) = 0\}.$$

$$\text{Then } SO(3)K(\theta)\mathcal{S} = K(\theta).$$

We consider a martensitic phase transformation that takes place at the temperature θ_c, with the lattice being cubic (fcc or bcc) for $\theta \geq \theta_c$.

This is described by a change of shape of the lattice with respect to the lattice $\mathbf{B}$ at θ_c given by $\mathbf{U}(\theta) = \mathbf{U}(\theta)^T > 0$.

(Note that by the polar decomposition theorem we can write any $\mathbf{A} \in GL^+(3, \mathbb{R})$ in the form $\mathbf{A} = \mathbf{RU}$ with $\mathbf{R} \in SO(3)$, $\mathbf{U} = \mathbf{U}^T > 0$, so that we can always describe the change of shape by such a $\mathbf{U}$.)

Thus we assume that

$$K(\theta) = \begin{cases} \alpha(\theta) SO(3)\mathcal{S} & \theta > \theta_c \\ SO(3)\mathcal{S} \cup SO(3)\mathbf{U}(\theta_c)\mathcal{S} & \theta = \theta_c \\ SO(3)\mathbf{U}(\theta)\mathcal{S} & \theta < \theta_c \end{cases},$$

where $\alpha(\theta) > 0$ gives the thermal expansion of the cubic lattice, with $\alpha(\theta_c) = 1$.