1. INTRODUCTION TO SPACE-GROUP SYMMETRY

\[ \mathbf{v} \cdot \mathbf{w} = (x_1 y_1 z_1) \cdot \mathbf{G} \cdot \left( \begin{array}{c} x_2 \\ y_2 \\ z_2 \end{array} \right) \]

From this it follows how the metric tensor transforms under a basis transformation \( \mathbf{P} \). If \((a', b', c') = (a, b, c)P\), then the metric tensor \( \mathbf{G}' \) of \( \mathbf{L} \) with respect to the new basis \( a', b', c' \) is given by

\[ \mathbf{G}' = \mathbf{P}^T \cdot \mathbf{G} \cdot \mathbf{P}. \]

An alternative way to specify the geometry of a lattice in \( \mathbb{R}^3 \) is using the cell parameters, which are the lengths of the lattice basis vectors and the angles between them.

Definition

For a lattice \( \mathbf{L} \) in \( \mathbb{R}^3 \) with lattice basis \( \mathbf{a}, \mathbf{b}, \mathbf{c} \) the cell parameters (also called lattice parameters, lattice constants or metric parameters) are given by the lengths

\[ a = |\mathbf{a}| = \sqrt{\mathbf{a} \cdot \mathbf{a}}, \quad b = |\mathbf{b}| = \sqrt{\mathbf{b} \cdot \mathbf{b}}, \quad c = |\mathbf{c}| = \sqrt{\mathbf{c} \cdot \mathbf{c}} \]

of the basis vectors and by the interaxial angles

\[ \alpha = \angle(\mathbf{b}, \mathbf{c}), \quad \beta = \angle(\mathbf{c}, \mathbf{a}), \quad \gamma = \angle(\mathbf{a}, \mathbf{b}). \]

Owing to the relation \( \mathbf{v} \cdot \mathbf{w} = |\mathbf{v}| |\mathbf{w}| \cos \angle(\mathbf{v}, \mathbf{w}) \) for the scalar product of two vectors, one can immediately write down the metric tensor in terms of the cell parameters:

\[ \mathbf{G} = \begin{pmatrix} a^2 & ab \cos \gamma & ac \cos \beta \\ ab \cos \gamma & b^2 & bc \cos \alpha \\ ac \cos \beta & bc \cos \alpha & c^2 \end{pmatrix}. \]

1.3.2.3. Unit cells

A lattice \( \mathbf{L} \) can be used to subdivide \( \mathbb{R}^3 \) into cells of finite volume which all have the same shape. The idea is to define a suitable subset \( \mathbf{C} \) of \( \mathbb{R}^3 \) such that the translates of \( \mathbf{C} \) by the vectors in \( \mathbf{L} \) cover \( \mathbb{R}^3 \) without overlapping. Such a subset \( \mathbf{C} \) is called a unit cell of \( \mathbf{L} \), or, in the more mathematically inclined literature, a fundamental domain of \( \mathbb{R}^3 \) with respect to \( \mathbf{L} \). Two standard constructions for such unit cells are the primitive unit cell and the Voronoi domain (which is also known by many other names).

Definition

Let \( \mathbf{L} \) be a lattice in \( \mathbb{R}^3 \) with lattice basis \( \mathbf{a}, \mathbf{b}, \mathbf{c} \).

(i) The set \( \mathbf{C} := \{ \mathbf{v} + \mathbf{w} + \mathbf{z} | 0 \leq x, y, z < 1 \} \) is called the primitive unit cell of \( \mathbf{L} \) with respect to the basis \( \mathbf{a}, \mathbf{b}, \mathbf{c} \). The primitive unit cell is the parallelepiped spanned by the vectors of the given basis.

(ii) The set \( \mathbf{C} := \{ \mathbf{w} | |\mathbf{w}| \leq |\mathbf{w} - \mathbf{v}| \} \) for all \( \mathbf{v} \in \mathbf{L} \) is called the Voronoi domain or Dirichlet domain or Wigner–Seitz cell or Wirkungsbereich or first Brillouin zone (for the case of reciprocal lattices in dual space, see Section 1.3.2.5) of \( \mathbf{L} \) (around the origin). The Voronoi domain consists of those points of \( \mathbb{R}^3 \) that are closer to the origin than to any other lattice point of \( \mathbf{L} \). See Fig. 1.3.2.2 for examples of these two types of unit cells in two-dimensional space.

It should be noted that the attribute ‘primitive’ for a unit cell is often omitted. The term ‘unit cell’ then either denotes a primitive unit cell in the sense of the definition above or a slight generalization of this, namely a cell spanned by vectors \( \mathbf{a}, \mathbf{b}, \mathbf{c} \) which are not necessarily a lattice basis. This will be discussed in detail in the next section. If a unit cell in the even more general sense of a cell whose translates cover the whole space without overlap (thus including e.g. Voronoi domains) is meant, this should be indicated by the context.

The construction of the Voronoi domain is independent of the basis of \( \mathbf{L} \), as the Voronoi domain is bounded by planes bisecting the line segment between the origin and a lattice point and perpendicular to this segment. In two-dimensional space, the Voronoi domain is simply bounded by lines, in three-dimensional space it is bounded by planes and more generally it is bounded by \((n-1)\)-dimensional hyperplanes in \(n\)-dimensional space.

The boundaries of the Voronoi domain and its translates overlap, thus in order to get a proper fundamental domain, part of the boundary has to be excluded from the Voronoi domain.

The volume \( V \) of the unit cell can be expressed both via the metric tensor and via the cell parameters. One has

\[ V^2 = \det \mathbf{G} = a^2 b^2 c^2 (1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma). \]

and thus

\[ V = abc \sqrt{1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma}. \]

Although the cell parameters depend on the chosen lattice basis, the volume of the unit cell is not affected by a transition to a different lattice basis \( a', b', c' \). As remarked in Section 1.3.2.1, two lattice bases are related by an integral basis transformation \( \mathbf{P} \) of determinant \( \pm 1 \) and therefore \( \det \mathbf{G}' = \det(\mathbf{P}^T \cdot \mathbf{G} \cdot \mathbf{P}) = \det \mathbf{G} \), i.e. the determinant of the metric tensor is the same for all lattice bases.

Assuming that the vectors \( \mathbf{a}, \mathbf{b}, \mathbf{c} \) form a right-handed system, the volume can also be obtained via

\[ V = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \times \mathbf{a}) = \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b}). \]

1.3.2.4. Primitive and centred lattices

The definition of a lattice as given in Section 1.3.2.1 states that a lattice consists precisely of the integral linear combinations of the vectors in a lattice basis. However, in crystallographic