6.6: Metric tensor

A metric tensor is used to measure distances in a space. In crystallography the spaces considered are vector spaces with *Euclidean* metrics, *i.e.*ones for which the rules of Euclidean geometry apply. In that case, given a basis $\mathbf{e_i}$ of a *Euclidean space*, E^n, the metric tensor is a rank 2 tensor the components of which are:

$$g_{ij} = \mathbf{e_i} \cdot \mathbf{e_j} = \mathbf{e_j} . \mathbf{e_i} = g_{ji}.$$

It is a symmetrical tensor. Using the metric tensor, the scalar product of two vectors, $\mathbf{x} = x^i \, \mathbf{e_i}$ and $\mathbf{y} = y^j \, \mathbf{e_j}$ is written:

$$\mathbf{x} \cdot \mathbf{y} = x^i \, \mathbf{e_i} \cdot y^j \, \mathbf{e_j} = g_{ij} \, x^i \, y^j.$$

In a three-dimensional space with basis vectors **a**, **b**, **c**, the coefficients g_{ij} of the metric tensor are:

$$g_{11} = \mathbf{a^2};\ g_{12} = \mathbf{a} \cdot \mathbf{b};\ g_{13} = \mathbf{a} \cdot \mathbf{c};$$
$$g_{21} = \mathbf{b} \cdot \mathbf{a};\ g_{22} = \mathbf{b^2};\ g_{23} = \mathbf{b} \cdot \mathbf{c};$$
$$g_{31} = \mathbf{c} \cdot \mathbf{a};\ g_{32} = \mathbf{c} \cdot \mathbf{b};\ g_{33} = \mathbf{c^2};$$

Because the metric tensor is symmetric, $g_{12} = g_{21}$, $g_{13} = g_{31}$, and $g_{13} = g_{31}$. Thus there are only six unique elements, often presented as

$$g_{11}\ g_{22}\ g_{33}$$
$$g_{23}\ g_{13}\ g_{12}$$

or, multiplying the second row by 2, as a so-called G^6 ("G" for Gruber) vector

$$(\ \mathbf{a^2}, \mathbf{b^2}, \mathbf{c^2}, 2\ \mathbf{b} \cdot \mathbf{c}, 2\ \mathbf{a} \cdot \mathbf{c}, 2\ \mathbf{a} \cdot \mathbf{b}\ )$$

The inverse matrix of g_{ij}, g^{ij}, ($g^{ik} g_{kj} = \delta^k_j$, Kronecker symbol, = 0 if $i \neq j$, = 1 if $i = j$) relates the dual basis, or reciprocal space vectors $\mathbf{e^i}$ to the direct basis vectors $\mathbf{e_i}$ through the relations:

$$\mathbf{e^j} = g^{ij}\ \mathbf{e_j}$$

In three-dimensional space, the dual basis vectors are identical to the reciprocal space vectors and the components of g^{ij} are:

$$g^{11} = \mathbf{a^{*2}};\ g^{12} = \mathbf{a^*} \cdot \mathbf{b^*};\ g^{13} = \mathbf{a^*} \cdot \mathbf{c^*};$$
$$g^{21} = \mathbf{b^*} \cdot \mathbf{a^*};\ g^{22} = \mathbf{b^{*2}};\ g^{23} = \mathbf{b^*} \cdot \mathbf{c^*};$$
$$g^{31} = \mathbf{c^*} \cdot \mathbf{a^*};\ g^{32} = \mathbf{c^*} \cdot \mathbf{b^*};\ g^{33} = \mathbf{c^{*2}};$$

with:

$$g^{11} = b^2 c^2 \sin^2 \alpha / \mathrm{V}^2;\ g^{22} = c^2 a^2 \sin^2 \beta / \mathrm{V}^2;\ g^{33} = a^2 b^2 \sin^2 \gamma / \mathrm{V}^2;$$

$g^{12} = g^{21} = (abc^2/ \mathrm{V}^2)(\cos\alpha \cos\beta - \cos\gamma)$; $g^{23} = g^{32} = (a^2bc/ \mathrm{V}^2)(\cos\beta \cos\gamma - \cos\alpha)$; $g^{31} = g^{13} = (ab^2c/ \mathrm{V}^2)(\cos\gamma \cos\alpha - \cos\beta)$

where V is the volume of the unit cell (**a**, **b**, **c**).

Change of basis

In a change of basis the direct basis vectors and coordinates transform like:

$$\mathbf{e'_j} = A_j^{\ i}\ \mathbf{e_i};\ x'^j = B_i^{\ j}\ x^{\ i},$$

where $A_j^{\ i}$ and $B_i^{\ j}$ are transformation matrices, transpose of one another. According to their definition, the components g_{ij}, of the metric tensor transform like products of basis vectors:

$$g'_{kl} = A_k^{\ i} A_l^{\ j} g_{ij}.$$

They are the doubly covariant components of the metric tensor.

The dual basis vectors and coordinates transform in the change of basis according to:

$$\mathbf{e'^j} = B_i^{\ j}\ \mathbf{e^i};\ x'_j = A_j^{\ i} x_i,$$

and the components g^{ij} transform like products of dual basis vectors:

$g'^{kl} = A_i^{\ k}\ A_j^{\ l}\ g^{ij}$.

They are the doubly contravariant components of the metric tensor.

The mixed components, $g^i{}_j = \delta^i{}_j$, are once covariant and once contravariant and are invariant.

Properties of the metric tensor

- The **tensor nature** of the metric tensor is demonstrated by the behaviour of its components in a change of basis. The components g_{ij} andg^{ij} are the components of a *unique* tensor.
- The **squares of the volumes** V and V^* of the direct space and reciprocal space unit cells are respectively equal to the determinants of theg_{ij} 's and the g^{ij} 's:

$V^2 = \Delta (g_{ij}) = abc(1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \alpha \cos \alpha)$

$V^{*2} = \Delta (g^{ij}) = 1/ V^2$.

- One changes the **variance of a tensor** by taking the contracted tensor product of the tensor by the suitable form of the metric tensor. For instance:

$g_{im} t^{ij..}{}_{kl..} = t^{j..}{}_{klm..}$

Multiplying by the doubly covariant form of the metric tensor increases the covariance by one, multiplying by the doubly contravariant form increases the contravariance by one.

See also

- Section 1.1.3 of *International Tables of Crystallography, Volume B*
- Section 1.1.2 of *International Tables of Crystallography, Volume D*

Contributors

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