*Acta Cryst.* (1974). A**30**, 846

**On the concept of reciprocal basis vectors.** By T. Knudsen, *Concrete Research Laboratory, Karlstrup,* 2690 *Karlslunde, Denmark*

(*Received* 17 *May* 1974; *accepted* 3 *July* 1974)

Ewald's concept of reciprocal basis vectors can be defined in a more general way. It is suggested that the definition of these basis vectors should be presented within the framework of the matrix notation, and not lean so heavily on the concept of a skew product of vectors. The metric matrix, which bears significance in any vector space is the crucial matrix in such a definition.

The concept of a reciprocal basis set of vectors is of great significance in crystallography. Here, often called reciprocal space, this concept helps to bring about a condensed way of representing the laws of diffraction. From the lattice-vectors $\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3$, the reciprocal basis-vectors $\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3$ are derived by the following definitions:

$$\mathbf{b}_1=\frac{\mathbf{a}_2\times\mathbf{a}_3}{\mathbf{a}_1\cdot\mathbf{a}_2\times\mathbf{a}_3}\,;\quad \mathbf{b}_2=\frac{\mathbf{a}_1+\mathbf{a}_3}{\mathbf{a}_1\cdot\mathbf{a}_2\times\mathbf{a}_3}\,;\quad \mathbf{b}_3=\frac{\mathbf{a}_1\times\mathbf{a}_2}{\mathbf{a}_1\cdot\mathbf{a}_2\times\mathbf{a}_3}\,. \tag{1}$$

This definition, commonly seen in textbooks on the subject, guaranties the orthonormality conditions:

$$\mathbf{b}_i\cdot\mathbf{a}_j=\delta_{ij}\,, \tag{2}$$

$\delta_{ij}$ being the Kroenecker delta.

By virtue of this definition, the inner or scalar product of two vectors $\mathbf{f}$ and $\mathbf{v}$ can be written

$$\mathbf{f}\cdot\mathbf{v}=f_1'\cdot v_1+f_2'\cdot v_2+f_3'\cdot v_3 \tag{3}$$

where primed and unprimed symbols refer to the components in the reciprocal and lattice bases respectively.

Definition (1) of a reciprocal basis, leans on the concept of a vector, or skew product: $\mathbf{a}_i\times\mathbf{a}_j$. Thus when defining the reciprocal basis in a two-dimensional lattice, one has to make use of a vector perpendicular to the plane, in order to apply definition (1) in this two-dimensional case.

In our opinion the concept of reciprocal basis-vectors in crystallography should be handled in accordance with the more general definition of a reciprocal basis.

Consider the set of basis vectors:

$$\mathbf{a}_1,\mathbf{a}_2,\ldots\mathbf{a}_i\ldots\mathbf{a}_n,$$

these being vectors in a quite general sense, and let us confine ourselves to real vectors in what is to follow.

If these basis vectors are all linearly independent, one can construct the metric matrix of rank $n$, given the definition of the inner product of two vectors:

$$M_{ij}=\mathbf{a}_i\cdot\mathbf{a}_j\,.$$

For vectors in three-dimensional Euclidian space, this is done according to the well known rule:

$$\mathbf{a}_i\cdot\mathbf{a}_j=|a_i|\cdot|a_j|\cdot\cos\theta$$

where $\theta$ is the angle between the two vectors.

For function vectors, functions of the set $\tau$ of independent variables, defined in the interval $[\tau_1,\tau_2]$, this definition might read:

$$\mathbf{a}_i\cdot\mathbf{a}_j=\int_{\tau 1}^{\tau 2}a_i(\tau)\cdot a_j(\tau)\mathrm{d}\tau\,.$$

For any kind of inner product the metric matrix is constructed by:

$$\mathbf{M}=\begin{pmatrix}M_{11}\ldots M_{1n}\\ \cdot\ \ \cdots\cdot\\ \cdot\ \ \cdots\cdot\\ \cdot\ \ \ \cdot\\ M_{n1}\ldots M_{nn}\end{pmatrix}=\begin{pmatrix}\mathbf{a}_1\cdot\mathbf{a}_1\ldots\mathbf{a}_1\cdot\mathbf{a}_n\\ \cdot\ \ \cdots\cdot\\ \cdot\ \ \ \cdot\ \cdot\\ \cdot\ \ \ \cdot\\ \mathbf{a}_n\cdot\mathbf{a}_1\ldots\mathbf{a}_n\cdot\mathbf{a}_n\end{pmatrix}. \tag{4}$$

For the special case of an orthonormal basis the metric matrix $\mathbf{M}$ is the identity matrix $\mathbf{I}$. In the language of matrices a vector is represented as a row or column matrix. In this representation of the calculus of vectors, the metric matrix is of the greatest significance.

Consider the representation of the inner product of two vectors $\mathbf{f}$ and $\mathbf{v}$ (the order of multiplication being immaterial for real vectors):

$$\begin{aligned}\mathbf{f}\cdot\mathbf{v}&=(f_1\cdot\mathbf{a}_1+f_2\cdot\mathbf{a}_2+\ldots f_n\cdot\mathbf{a}_n)\,.\\ &\qquad(v_1\cdot\mathbf{a}_1+v_2\cdot\mathbf{a}_2+\ldots v_n\cdot\mathbf{a}_n)\\ &=(f_1f_2\ldots f_n)\begin{pmatrix}\mathbf{a}_1\\ \mathbf{a}_2\\ \cdot\\ \cdot\\ \mathbf{a}_n\end{pmatrix}(\mathbf{a}_1\mathbf{a}_2\ldots\mathbf{a}_n)\begin{pmatrix}v_1\\ v_2\\ \cdot\\ \cdot\\ v_n\end{pmatrix}\\ &=(f_1f_2\ldots f_n)\begin{pmatrix}\mathbf{a}_1\,.\,\mathbf{a}_1\ldots\mathbf{a}_1\,.\,\mathbf{a}_n\\ \cdot\\ \cdot\\ \cdot\\ \mathbf{a}_n\,.\,\mathbf{a}_1\ldots\mathbf{a}_n\mathbf{a}_n\end{pmatrix}\begin{pmatrix}v_1\\ v_2\\ \cdot\\ \cdot\\ v_n\end{pmatrix}\\ &=\mathbf{F\,M\,V},\end{aligned} \tag{5}$$

where $\mathbf{F}$ is the row-matrix representing $\mathbf{f}$ and $\mathbf{V}$ the column-matrix representing $\mathbf{v}$.

The norm of a vector $\mathbf{f}$ is given by:

$$(\mathbf{f}\cdot\mathbf{f})^{1/2}=(\mathbf{FMF})^{1/2}\,.$$

The form of these representations of an inner product and the fact that $\mathbf{M}$ is generally different from the identity matrix, is the crucial point in the idea of a reciprocal basis. The reciprocal basis tries to maintain the simpler representation of an inner product which is found for the orthonormal basis.

$$\mathbf{f}\cdot\mathbf{v}=\mathbf{FMV}=\mathbf{FIV}=(f_1\cdot v_1+f_2\cdot v_2+\ldots f_n\cdot v_n)\,. \tag{6}$$

Consider now the basis shift:

$$\begin{pmatrix}\mathbf{b}_1\\ \mathbf{b}_2\\ \cdot\\ \cdot\\ \mathbf{b}_n\end{pmatrix}=\mathbf{M}^{-1}\begin{pmatrix}\mathbf{a}_1\\ \mathbf{a}_2\\ \cdot\\ \cdot\\ \mathbf{a}_n\end{pmatrix}. \tag{7}$$

In this new basis the **f** vector has the components $f'_1 f'_2 \ldots f'_n$ found by the transformation

$$(f'_1 f'_2 \ldots f'_n) = (f_1 f_2 \ldots f_n)\mathbf{M}\,. \tag{8}$$

Now it is obvious from the form (5) that with the help of this new basis $\mathbf{b}_1\,\mathbf{b}_2 \ldots \mathbf{b}_n$, the inner product can be written:

$$\mathbf{f}\cdot\mathbf{v} = \mathbf{F}'\mathbf{V} = (f'_1 \cdot v_1 + f'_2 \,.\, v_2 + \ldots f'_n \cdot v_n) \tag{9}$$

or for the length or the norm of the vector:

$$(\mathbf{f}\cdot\mathbf{f})^{1/2} = (f'_1 \cdot f_2 + f'_2 \cdot f_2 + \ldots f'_n \cdot f_n)^{1/2}\,. \tag{10}$$

To conclude, we state the fact that in any given vector space a reciprocal basis can be constructed with the help of the metric matrix. This reciprocal basis can be used to conserve the form (9) of an inner product. For a linear operator $\hat{P}$ it conserves the form of the matrix-element in the representation of this operator, namely:

$$P_{ij} = \mathbf{b}_i \cdot (\hat{P}\mathbf{a}_j)\,. \tag{11}$$

For the three-dimensional Euclidian space it can easily be verified that definition (7) is equivalent to definition (1). The difference is that definition (7) does not need the concept of a skew product of vectors, a concept which loses significance in spaces of more or fewer dimensions.

*Acta Cryst.* (1974). A**30**, 847

## Coherent neutron scattering amplitudes.

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(*Received* 28 *May* 1974; *accepted* 28 *May* 1974)

A list is given which summarizes additions and significant changes which have been reported since the publication of a full list of scattering amplitudes in 1972 [*Acta Cryst.* (1972). A**28**, 357–358].

In Table 1 are listed additions and significant changes which have been reported since the publication of a full list of scattering amplitudes by Bacon (1972).

Table 1. *Coherent scattering amplitudes*

| $Z$ | Element for Isotope | $b$ ($10^{-12}$ cm) | Reference |
|---|---|---|---|
| 7 | $^{15}$N | 0·65 | Kuznietz & Wedgwood (1972). |
| 12 | $^{24}$Mg | 0·55 | Abul Khail, Amin, Al-Naimi, Al-Saji, Al-Shahery, Petrunin & Zemlyanov (1972). |
| | $^{25}$Mg | 0·36 | |
| | $^{26}$Mg | 0·49 | |
| 52 | Te | 0·58 | Lindqvist & Lehmann (1973). |
| 60 | Nd | 0·75 | Schobinger-Papamentellos, Fischer, Vogt & Kaldis (1973). |
| 62 | $^{154}$Sm | 0·96 | Koehler & Moon (1972). |
| 63 | Eu | 0·68 at $\lambda = 1{\cdot}067$<br>0·61 at $\lambda = 0{\cdot}75$ Å | W. C. Koehler & J. W. Cable (unpublished). |
| 64 | $^{160}$Gd | 0·915 | Koehler, Moon, Cable & Child (1972). |
| 91 | $^{231}$Pa | $1{\cdot}3 \pm 0{\cdot}2$ | Wedgwood & Burlet (1974). |
| 95 | $^{243}$Am | 0·76 | Mueller, Lander & Reddy (1974). |
| 96 | $^{244}$Cm | ~0·7 | |

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