the above-mentioned point space but also to introduce simultaneously a *vector space* which is closely connected with the point space. Crystallographers are used to working in both spaces: crystal structures are described in point space, whereas face normals, translation vectors, Patterson vectors and reciprocal-lattice vectors are elements of vector spaces.

In order to carry out crystallographic calculations it is necessary to have a *metrics* in point space. Metrical relations, however, are most easily introduced in vector space by defining scalar products between vectors from which the length of a vector and the angle between two vectors are derived. The connection between the vector space $\mathbf{V}^n$ and the point space E^n transfers both the metrics and the dimension of $\mathbf{V}^n$ onto the point space E^n in such a way that distances and angles in point space may be calculated.

The connection between the two spaces is achieved in the following way:

(i) To any two points P and Q of the point space E^n a vector $\overrightarrow{PQ} = \mathbf{r}$ of the vector space $\mathbf{V}^n$ is attached.

(ii) For each point P of E^n and each vector $\mathbf{r}$ of $\mathbf{V}^n$ there is exactly one point Q of E^n for which $\overrightarrow{PQ} = \mathbf{r}$ holds.

(iii) $\overrightarrow{PQ} + \overrightarrow{QR} = \overrightarrow{PR}$.

The distance between two points P and Q in point space is given by the length $|\overrightarrow{PQ}| = (\overrightarrow{PQ}, \overrightarrow{PQ})^{1/2}$ of the attached vector $\overrightarrow{PQ}$ in vector space. In this expression, $(\overrightarrow{PQ}, \overrightarrow{PQ})$ is the scalar product of $\overrightarrow{PQ}$ with itself.

The angle determined by P, Q and R with vertex Q is obtained from

$$\cos(P, Q, R) = \cos(\overrightarrow{QP}, \overrightarrow{QR}) = \frac{(\overrightarrow{QP}, \overrightarrow{QR})}{|\overrightarrow{QP}| \cdot |\overrightarrow{QR}|}.$$

Here, $(\overrightarrow{QP}, \overrightarrow{QR})$ is the scalar product between $\overrightarrow{QP}$ and $\overrightarrow{QR}$. Such a point space is called an n-dimensional *Euclidean space*.

If we select in the point space E^n an arbitrary point O as the *origin*, then to each point X of E^n a unique vector $\overrightarrow{OX}$ of $\mathbf{V}^n$ is assigned, and there is a one-to-one correspondence between the points X of E^n and the vectors $\overrightarrow{OX}$ of $\mathbf{V}^n : X \leftrightarrow \overrightarrow{OX} = \mathbf{x}$.

Referred to a vector basis $\mathbf{a}_1, \ldots, \mathbf{a}_n$ of $\mathbf{V}^n$, each vector $\mathbf{x}$ is uniquely expressed as $\mathbf{x} = x_1\mathbf{a}_1 + \ldots + x_n\mathbf{a}_n$ or, using matrix multiplication,* $\mathbf{x} = (\mathbf{a}_1, \ldots, \mathbf{a}_n)\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$.

Referred to the coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$ of E^n, Fig. 8.1.2.1, each point X is uniquely described by the column of coordinates

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}.$$

Thus, the real numbers x_i are either the *coefficients of the vector* $\mathbf{x}$ of $\mathbf{V}^n$ or the *coordinates of the point* X of E^n.

* For this volume, the following conventions for the writing of vectors and matrices have been adopted:

(i) point coordinates and vector coefficients are written as $(n \times 1)$ column matrices;

(ii) the vectors of the vector basis are written as a $(1 \times n)$ row matrix;

(iii) *all* running indices are written as subscripts.

It should be mentioned that other conventions are also found in the literature, *e.g.* interchange of row and column matrices and simultaneous use of subscripts and superscripts for running indices.

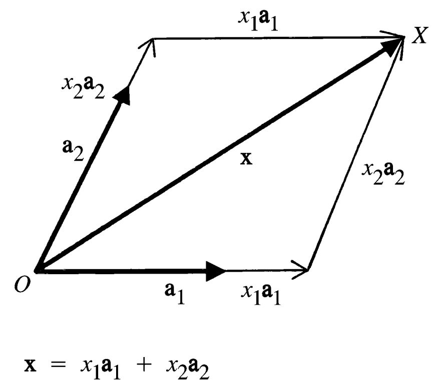

Fig. 8.1.2.1. Representation of the point X with respect to origin O by the vector $\overrightarrow{OX} = \mathbf{x}$. The vector $\mathbf{x}$ is described with respect to the vector basis $\{\mathbf{a}_1, \mathbf{a}_2\}$ of $\mathbf{V}^2$ by the coefficients x_1, x_2. The coordinate system $(O, \mathbf{a}_1, \mathbf{a}_2)$ of the point space E^2 consists of the point O of E^2 and the vector basis $\{\mathbf{a}_1, \mathbf{a}_2\}$ of $\mathbf{V}^2$.

An instruction assigning uniquely to each point X of the point space E^n an 'image' point $\tilde{X}$, whereby all distances are left invariant, is called an *isometry*, an *isometric mapping* or a *motion* M of E^n. Motions are invertible, *i.e.*, for a given motion $\mathsf{M} : X \to \tilde{X}$, the inverse motion $\mathsf{M}^{-1} : \tilde{X} \to X$ exists and is unique.

Referred to a coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$, any motion $X \to \tilde{X}$ may be described in the form

$$\begin{array}{ccccccc} \tilde{x}_1 & = & W_{11}x_1 & + \ldots + & W_{1n}x_n & + & w_1 \\ \vdots & = & \vdots & & \vdots & & \vdots \\ \tilde{x}_n & = & W_{n1}x_1 & + \ldots + & W_{nn}x_n & + & w_n. \end{array}$$

In matrix formulation, this is expressed as

$$\begin{pmatrix} \tilde{x}_1 \\ \vdots \\ \tilde{x}_n \end{pmatrix} = \begin{pmatrix} W_{11} & \ldots & W_{1n} \\ \vdots & & \vdots \\ W_{n1} & \ldots & W_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} + \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix}$$

or, in abbreviated form, as $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$, where $\tilde{\boldsymbol{x}}$, $\boldsymbol{x}$ and $\boldsymbol{w}$ are all $(n \times 1)$ columns and $\boldsymbol{W}$ is an $(n \times n)$ square matrix. One often writes this in even more condensed form as $\tilde{\boldsymbol{x}} = (\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x}$, or $\tilde{\boldsymbol{x}} = (\boldsymbol{W}|\boldsymbol{w})\boldsymbol{x}$; here, $(\boldsymbol{W}|\boldsymbol{w})$ is called the *Seitz symbol*.

A motion consists of a *rotation part* or *linear part* and a *translation part*. If the motion is represented by $(\boldsymbol{W}, \boldsymbol{w})$, the matrix $\boldsymbol{W}$ describes the rotation part of the motion and is called the *matrix part* of $(\boldsymbol{W}, \boldsymbol{w})$. The column $\boldsymbol{w}$ describes the translation part of the motion and is called the *vector part* or *column part* of $(\boldsymbol{W}, \boldsymbol{w})$. For a given motion, the matrix $\boldsymbol{W}$ depends only on the choice of the basis vectors, whereas the column $\boldsymbol{w}$ in general depends on the choice of the basis vectors *and* of the origin O; *cf.* Section 8.3.1.

It is possible to combine the $(n \times 1)$ column and the $(n \times n)$ matrix representing a motion into an $(n+1) \times (n+1)$ square matrix which is called the *augmented matrix*. The system of equations $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$ may then be expressed in the following form:

$$\left(\begin{array}{c} \tilde{x}_1 \\ \vdots \\ \tilde{x}_n \\ \hline 1 \end{array}\right) = \left(\begin{array}{ccc|c} & & & w_1 \\ & \boldsymbol{W} & & \vdots \\ & & & w_n \\ \hline 0 & \ldots & 0 & 1 \end{array}\right) \left(\begin{array}{c} x_1 \\ \vdots \\ x_n \\ \hline 1 \end{array}\right)$$

or, in abbreviated form, by $\tilde{\mathbb{x}} = \mathbb{W}\mathbb{x}$. The augmentation is done in two steps. First, the $(n \times 1)$ column $\boldsymbol{w}$ is attached to the $(n \times n)$ matrix and then the matrix is made square by attaching the $[1 \times (n+1)]$ row $(0 \ldots 0\ 1)$. Similarly, the $(n \times 1)$ columns $\boldsymbol{x}$ and $\tilde{\boldsymbol{x}}$

references