

FIG. 5 is a block diagram of analytical electron microscope apparatus according to the present invention for identifying an unknown material.

FIG. 6 is a flow chart of a preferred method of data collection and analysis performed by the apparatus of FIG. 5 according to the present invention.

FIG. 7 is a more detailed flow chart of a preferred embodiment of step 130 in FIG. 6.

FIG. 8 is a block diagram of automated diffractometry apparatus according to the present invention for symmetry analysis of a lattice structure.

FIG. 9 is a flow chart of a preferred method of data collection and analysis performed by the apparatus of FIG. 8.

FIG. 10 is a more detailed flow chart of a preferred embodiment of step 950 in FIG. 9.

FIG. 11 is a more detailed flow chart of a first embodiment of step 960 in FIG. 9.

FIG. 12 is a more detailed flow chart of a second embodiment of step 960 in FIG. 9.

FIG. 13 is a more detailed flow chart of a third embodiment of step 960 in FIG. 9.

FIG. 14 is a more detailed flow chart of a first embodiment of step 1100 in FIGS. 12 and 13.

FIG. 15 is a more detailed flow chart of a second embodiment of step 1100 in FIGS. 12 and 13.

DETAILED DESCRIPTION OF THE PREFERRED EMBODIMENTS

Referring to FIG. 1, a primitive or conventional unit cell of a lattice structure, which cell reflects all of the properties of the lattice structure, is defined by six parameters, namely three cell edges a, b and c, and three cell angles α , β and γ , as shown. In accordance with the present invention, the relationship between any two lattice structures, and the symmetry characteristics of a single lattice structure, can be determined by calculating in the following manner all 3×3 transformation matrices H (if any) which have elements that are integers or simple rational numbers, and which relate the two lattice cell structures (or the lattice structure to itself) to within specified tolerances of the lattice cell parameters. In other words cell Y=(H-Matrix) Z. The transformation relationship can be represented as

$$\begin{array}{l} \text{CELL Y} \\ Y_a \\ Y_b \\ Y_c \\ Y_\alpha \\ Y_\beta \\ Y_\gamma \end{array} \quad \begin{array}{l} \text{H Matrix} \\ \\ \\ \\ \\ \\ \\ \end{array} \quad \begin{array}{l} \text{CELL Z} \\ Z_a \\ Z_b \\ Z_c \\ Z_\alpha \\ Z_\beta \\ Z_\gamma \end{array} = \begin{array}{l} \\ \\ \begin{bmatrix} h_{11} & h_{12} & h_{13} \\ h_{21} & h_{22} & h_{23} \\ h_{31} & h_{32} & h_{33} \end{bmatrix} \\ \\ \\ \\ \\ \end{array}$$

Referring to FIG. 2, a preferred form of the converse transformation matrix generation method of the present invention which is adapted for computer implementation will be described with reference to two primitive cells Y and Z, which can be the same cell if a symmetry analysis is being performed on a lattice structure. It will also be appreciated that when an unknown lattice structure is being identified, one of the cells may be derived from a database or the like of known lattice structures. In that case, cell Y defines a known lattice structure in the database, and cell Z defines the unknown lattice structure. Further, in the following description, the cell edge parameters a, b and c of cells Y and Z will be referred to as YA, YB, YC and ZA, ZB, ZC, respectively; the cell angle parameters α , β and γ of the cells

will be similarly referred to as YAL, YBE, YGA and ZAL, ZBE and ZGA, respectively. The maximum tolerances acceptable (input parameters) for relating transformed CELL Z to CELL Y will be referred to as TOLI1, TOLI2, TOLI3, TOLI4, TOLI5, TOLI6, respectively; whereas the actual tolerances found when relating transformed CELL Z to CELL Y will be referred to as TOLA, TOLB, TOLC, TOLAL, TOLBE, and TOLGA, respectively. By definition these actual tolerances constitute the tolerance matrix T:

$$T = \begin{array}{l} \text{tol } a \quad \text{tol } b \quad \text{tol } c \\ \text{tol } \alpha \quad \text{tol } \beta \quad \text{tol } \gamma \end{array}$$

The first step 10 of the transformation matrix generation method of the present invention is to establish the edge and angle parameters YA, YB, YC, YAL, YBE, YGA ZA, AB, ZC, ZAL, ZBE and ZGA of cells Y and Z, and to define the maximum acceptable tolerance values TOLI1, TOLI2, TOLI3, TOLI4, TOLI5 and TOLI6. It will be appreciated that the primitive cell parameters for an unknown lattice structure Z can be experimentally measured using conventional techniques, such as x-ray diffractometry or analytical electron microscopy, for example. One preferred way to obtain cell parameter data for an unknown lattice structure is to determine two planes of diffraction data in reciprocal space. From the data on each plane and from the orientation of the two planes with respect to each other, a primitive cell in reciprocal space can be determined. The cell is then converted to direct space in Ångstrom units. Advantageously, the unknown lattice cell Z also is reduced in a conventional manner. Further, a reduced form of cell Y as well as cell Z is advantageously used. The use of reduced cells speeds computer processing and limits the matrix elements which need to be considered. As noted above, it is not necessary or even advantageous to determine a standard cell. Further, if the cell determined is not a primitive cell, but instead a supercell in reciprocal space (subcell in direct space) because diffraction nodes were missed, analysis of the lattice structure can still be carried out using the matrix approach of the present invention.

Maximum tolerance values are selected according to an assessment of the size of the experimental errors. By setting large limits (e.g., 1.0 and 6.0 for the cell edges and angles, respectively), all possible lattice relationships/symmetries may be obtained. It will be appreciated that the cell parameter and maximum tolerance values are stored as data in a computer for computer implementation of the transformation matrix generation method of the present invention.

The next step (step 20 in FIG. 2) is to calculate the dot products Z11, Z22, Z33, Z23, Z13 and Z12 for cell Z (i.e., A.A, B.B, C.C, B.C, A.C and A.B), as follows:

$$\begin{array}{l} Z_{11} = Z_A * Z_A \\ Z_{22} = Z_B * Z_B \\ Z_{33} = Z_C * Z_C \\ Z_{23} = Z_B * Z_C * \cos(ZAL/RADIAN) \\ Z_{13} = Z_A * Z_C * \cos(ZBE/RADIAN) \\ Z_{12} = Z_A * Z_B * \cos(ZGA/RADIAN) \end{array}$$

where RADIAN = $360/2\pi$.

In step 30, all of the matrix triples AU, AV, AW; BU, BV, BW; and CU, CV; CW are respectively determined