

A portion of the present invention's matrix approach to lattice analysis in the context of determining symmetry has been discussed in detail by the present applicants in their article "A Matrix Approach to Symmetry", *Acta Cryst.* (1987) A43, pp. 375-384, which is hereby incorporated by reference. However, no method for generating the necessary symmetry matrices which relate any observed primitive cell of a lattice to itself is described in the aforesaid article, or in any other published article. The general converse transformation method described herein which applicants have developed generates matrices relating any two lattice cells (including a lattice cell to itself); and can be used in new, more efficacious methods for control of diffractometers, and for phase identification using analytical electron microscope (AEM) data and existing large scale databases providing chemical, physical and crystallographic data on solid-state materials.

Accordingly, it is a primary object of the present invention to provide apparatus and methods for identifying lattice structures using the converse transformation matrix generation method of the present invention.

It is a further primary object of the present invention to provide apparatus and methods for identifying unknown materials using electron diffraction and energy dispersive spectroscopy data, databases on solid-state materials and the converse transformation matrix generation method of the present invention.

It is a still further primary object of the present invention to provide improved diffractometry apparatus and methods using the converse transformation matrix generation method of the present invention.

In accordance with the present invention, a method of comparing two crystalline materials to determine whether they have a predetermined lattice structure relationship therebetween comprises the steps of:

a) determining primitive lattice cells Y and Z, respectively, for the two materials, the cells Y and Z having three cell edges YA, YB, YC and ZA, ZB and ZC, respectively, and three cell angles YAL, YBE, YGA and ZAL, ZBE and ZGA, respectively;

b) generating all matrices H, if any, which transform cell Z into cell Y within predetermined maximum cell edge and angle tolerances TOL11, TOL12, TOL13, and TOL14, TOL15, TOL16, respectively; and if at least one matrix H is generated;

c) analyzing the nature of the generated matrix (matrices) H and its inverse (their respective inverses) H' to determine the nature of the lattice relationship:

1) If a matrix H has integer matrix elements and a determinant HDET = 1, then Cell Z and Cell Y define the same lattice;

2) If a matrix H or its inverse H' has integer matrix elements and a determinant HDET greater than one, then Cell Z and Cell Y are in a subcell/supercell relationship; or

3) If a matrix H and its inverse H' both have one or more fractional matrix elements, then Cell Z and Cell Y define lattices that are in a composite relationship.

In accordance with a further aspect of the present invention, a method for analyzing the symmetry of a crystalline material comprises the steps of:

a) collecting edge data ZA, ZB and ZC and angle data ZAL, ZBE and ZGA defining any primitive lattice cell Z of the material;

b) generating all symmetry matrices Hs which transform cell Z into itself within predetermined maximum cell edge and angle parameter tolerances TOL11,

TOL12, TOL13 and TOL14, TOL15, TOL16, respectively;

c) determining the metric symmetry using symmetry matrices Hs; and

d) defining the crystal symmetry using symmetry matrices Hs.

In accordance with a still further aspect of the present invention, a method for identifying an unknown crystalline material comprises the steps of;

a) determining a primitive lattice cell Z of the unknown material, the cell Z having three cell edges ZA, ZB, and ZC, respectively, and three cell angles ZAL, ZBE, and ZGA, respectively;

b) determining the chemical composition of the unknown material;

c) searching a database comprising lattice cell data and element type data for materials with known lattice structures and chemical compositions by at least in part generating matrices H identifying all compounds having lattice cell structures related to cell Z;

d) analyzing the matrices H to identify which of the compounds identified in step c) match cell Z by having a lattice cell structure identical to or in a subcell/supercell derivative relationship to cell Z, and saving the lattice cell matching compounds as a first data set;

e) searching the database for all compounds which match the unknown material by having the same element types as the unknown material, and saving the element type matching compounds as a second data set; and

f) combining the first and second data sets to derive all known compounds having the same lattice cell structure and element types.

In accordance with another aspect of the present invention, in each of the foregoing methods, the matrices H are generated by a converse transformation method comprising the steps of:

finding all matrix triples AU, AV, AW; BU, BV, BW; CU, CV, CW which accomplish transformation of the respective Z-cell edges to the corresponding edges of the desired cell within the corresponding ones of the maximum cell edge tolerances; and

finding all combinations of the matrix triples found in the matrix-triple-finding step which accomplish transformation of the respective Z-cell angles to the corresponding angles of the desired cell within the corresponding ones of the maximum acceptable cell angle tolerances.

These and other objects, features and advantages of the present invention will be described in or apparent from the following detailed description of preferred embodiments.

BRIEF DESCRIPTION OF THE DRAWING

The preferred embodiments will be described with reference to the drawing, in which:

FIG. 1 is a graphical representation of the parameters of a primitive cell of a lattice structure.

FIGS. 2A-2B are a flow chart of a preferred embodiment of the converse transformation matrix generation method of the present invention.

FIGS. 3A-3C are a more detailed flow chart of a preferred embodiment of step 60 shown in FIG. 2 which integrates steps 70 and 80 as part of step 60.

FIGS. 4A-4C are a more detailed flow chart of a preferred embodiment of step 30 shown in FIG. 2.