and the holohedry of cells 1 and 2 is defined by $\{H_1\}$ and $\{H_2\}$, respectively, where H_1 and H_2 are groups of symmetry matrices Hs. The relationship between the symmetry groups H_1 and H_2 is given by the equation $H_2=SH_1S^{-1}$. This equation defines the effect a change of basis has on the matrix of a linear operator. By definition, two matrices representing the same linear operator with respect to different bases are similar.

While the present invention has been described with reference to a particular preferred embodiment of the method and apparatus, the invention is not limited to the specific example given, and other embodiments will be apparent to those skilled in the art without departing from the spirit and scope of the invention.

What is claimed is:

1. Automatic apparatus for identifying an unknown crystalline material comprising:

a radiation generator for irridating a sample of the unknown material with radiation;

a radiation detector for detecting radiation received from the irridated sample and producing electrical output signals indicative of the detected radiation;

an electronic signal analyzer, responsive to said electrical output signals generated by said radiation detector, for producing electrical data signal outputs indicative of a primitive lattice cell Z of the unknown material, said cell Z having three cell edges ZA, AB and ZC, respectively, and three cell angles ZAL, ZBE, and ZGA, respectively;

a first computer accessible memory in which is stored a database comprising lattice cell data for materials with known lattice structures;

first computer search means responsive to said electronic signal analyzer data signal outputs for automatically searching said database using a converse transformation method to generate matrices H identifying all materials, if any, having lattice cell structures related to cell Z; and

computer means for analyzing any matrices H generated by said first search means to identify which of the database materials identified by the generated matrices H match cell Z by having a lattice cell structure identical to or in a subcell/supercell derivative relationship to cell Z, any database material so identified as matching cell Z constituting a possible identification of the unknown crystalline material.

2. The apparatus of claim 1 wherein a diffractometer constitutes said radiation generator and radiation detector.

3. The apparatus of claim 2 wherein said diffractometer is selected from the group consisting of an x-ray diffractometer which irradiates the sample of the unknown material with x-ray radiation, an electron diffractometer which irradiates the sample of the unknown material with electron radiation, and a neutron diffractometer which irradiates the sample of the unknown material with neutron radiation.

4. The apparatus of claim 2 wherein said signal analyzer further comprises a controller for controlling the orientation of the sample relative to said diffractometer.

5. The apparatus of claim 1 wherein an analytical electron microscope constitutes said radiation generator and radiation detector.

6. The apparatus of claim 1 wherein the materials with known lattice structures have chemical compositions, and said database further comprises element type data identifying the chemical compositions of the materials with known lattice structure, and said apparatus further comprises:

means for determining the element types identifying the chemical composition of the unknown material and producing electrical signal outputs indicative of the unknown material element types;

second computer search means responsive to the electrical signal outputs produced by said element type determining means for automatically searching said database for all compounds which match the unknown material by having the same or related element types as the unknown material;

a computer accessible second memory for saving as a first data set the compounds matching cell Z identified by said matrix H analyzing means, and as a second data set the matching compounds with the same element types as the unknown material identified by said second search means; and

said computer means includes means for combining said first and second data stored in said electronic memory to derive all known compounds having the same lattice cell structure and element types as the unknown material.

7. The apparatus of claim 6 wherein said means for determining element types comprises an energy dispersive x-ray spectrometer.

8. The apparatus of claim 1 wherein said first computer search means and said computer analyzing means cooperate to:

search said database without generating said matrices H to identify all compounds which match said cell Z with respect to cell edges;

determine derivative subcells and supercells of said cell Z;

search said database without generating said matrices H to identify all compounds which match said derivative subcells or supercells with respect to cell edges; and

search the compounds identified by said database searching using said converse transformation method to generate matrices H identifying those compounds which match cell Z with respect to both cell edges and cell angles.

9. The apparatus of claim 8 wherein:

the lattice cell data in said database is in the form of reduced cell data;

a reduced form of said cell Z is generated; and

the derivative subcells and supercells are produced in reduced form.

10. The apparatus of claim 1 wherein said converse transformation method comprises the steps of:

a) defining maximum acceptable cell edge and angle tolerances TOLI1, TOLI1, TOLI3 and TOLI4, TOLI5, TOLI6 for cell edges ZA AB and AC and cell angles ZAL, ZBE and ZGA, respectively, for the transformation of cell Z into another cell;

b) finding all matrix triples AU, AV, AW; BU, BV, BW; CU, CV, CW which accomplish transformation, within the corresponding ones of said maximum cell edge tolerances TOLI1, TOLI2 and TOLI3, of the respective Z-cell edges ZA, ZB, and ZC to corresponding edges of a database cell;

c) finding all combinations of said matrix triples found in said matrix-triple-finding step b) which accomplish transformation of the respective Z-cell angles to the corresponding angles of a database cell within the corresponding ones of said maxi-