Simply by inspecting the dependency relations obtained from the reduced row echelon form of the matrix, it can be determined whether a proper basis has been selected and, if not, which directions of the two-fold axes should have been chosen (step **1140**). Each of the six combinations of the two-fold axes in the tetragonal system leads to one of three recognizable types of matrices. Similarly, in the hexagonal system, each of the fifteen combinations of two-fold axes falls into one of four recognizable forms of matrices. When the reduced row echelon form of the matrix for the tetragonal or the hexagonal system is

order of axis

$$\begin{array}{c} \begin{matrix} 2 & 2 & 4 & 2 & 2 \end{matrix} \\ \begin{pmatrix} 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & -1 & 1 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} \end{array}$$

or

order of axis

$$\begin{array}{c} \begin{matrix} 2 & 2 & 6 & 2 & 2 & 2 & 2 \end{matrix} \\ \begin{pmatrix} 1 & 0 & 0 & 1 & -1 & 1 & -2 \\ 0 & 1 & 0 & -1 & -1 & 2 & -1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \end{array}$$

respectively, or its equivalent, the proper basis has been chosen.

Perhaps the easiest way to understand the dependency equations in the reduced row echelon form of the matrix is through use of a diagram For both the tetragonal and hexagonal systems, the vectors projected onto the ab plane are plotted and the respective figures are compared with those for space groups P4/mmm and P6/mmm in *International Tables For Crystallography* (1983). With a plot of the dependency equations, the vectors that have been chosen, and if necessary, which vectors should have been selected, can be readily visualized.

The analysis-of-dependency-equations method for selecting the directions of symmetry axes to be used as cell edges is similar in approach to the lattice method of obtaining a standard cell transformation matrix, as both methods use elementary row operations to reduce a matrix to a row echelon form. The lattice method may be viewed as a form of lattice reduction, whereas the analysis-of-dependency-equations method may be viewed as a form of symmetry reduction.

The determinant method (FIG. **15**) for selecting the directions of symmetry axes to be used as cell edges greatly simplifies the analysis based on symmetry because data is analyzed with respect to any orientation without having to view it, either visually or mathematically, from a standard basis. In the tetragonal system, there are six ways to combine two two-fold axes with a four-fold axis. Similarly, in the hexagonal system, there are fifteen ways to combine two two-fold axes with a six-fold axis. For each combination, a 3×3 matrix of directions is assembled (step **1150**). The determinants of these matrices are then calculated (step **1160**). The directions to be used for the cell edges are found directly from the values of the determinants of these matrices (step **1170**). In the tetragonal system, one of the six determinants will be twice the others. If the four possible two-fold axes are labelled 1, 2, 3, and 4, the combination of 1 and 2 with a four-fold axis gives a determinant twice the rest, and the vectors 3 and 4 should be selected as directions for the conventional cell edges. As another example, in the hexagonal system, there will be nine combinations with a determinant of ±1, three combinations with a determinant of ±2, and three combinations with a determinant of ±3. If the six possible two-fold axes are labelled 1–6, and the combinations of 1–2, 1–3, and 2–3 give determinants of ±3, then the directions for any two of the two-fold axes 4, 5 or 6 may be used as cell edges.

Often in carrying out practical or theoretical calculations in which symmetry is involved, it is convenient to shift basis systems. The matrix approach of the present invention permits groups of symmetry matrices to be obtained with respect to any selected basis. The values of the elements in each symmetry matrix depend on the kind and orientation of each symmetry operation with respect to the coordinate system chosen. As a result, the group of symmetry matrices generated from a skewed unit cell will be different from the group symmetry matrices generated from either a standard cell or a second skewed cell. Since any two cells defining the lattice belong to the same Bravais class, there exists a homogeneous linear transformation which will transform one lattice into the other and will transform the holohedry of one lattice into the holohedry of the other. The matrices may be calculated either directly using the reverse transformation method of the present invention; or by application of the similarity relationship, once the matrices are known with respect to any initial basis. The transformation of cell 1 to cell 2 is represented by the equation

$$\begin{pmatrix} a_2 \\ b_2 \\ c_2 \end{pmatrix} = S \begin{pmatrix} a_1 \\ b_1 \\ c_1 \end{pmatrix}$$

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:

an electronic signal analyzer, responsive to electrical signals generated by detecting radiation received from a sample of the unknown material which has been irradiated by radiation, 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, ZB and ZC, respectively, and three cell angles ZAL, ZBE and ZGA, respectively;

a first computer accessible memory in which is stored