APPARATUS AND METHODS FOR IDENTIFYING AND COMPARING LATTICE STRUCTURES AND DETERMINING LATTICE STRUCTURE SYMMETRIES

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BACKGROUND AND SUMMARY

This invention relates generally to apparatus and methods for identifying lattice structures, and more particularly to apparatus and methods for identifying intralattice and interlattice relationships.

A knowledge of the nature of the lattice structure of a material, as well as how it relates to the lattice structures of other materials, is essential in any systematic analysis of physical properties, and has many important commercial applications. For example, in crystallography, it is important for further analysis and identification of a crystalline structure under investigation to determine its symmetry characteristics. As another example, in materials design, once a new compound has been synthesized with a sought-after property, it can be extremely useful to the researcher to find all other materials that bear some specified lattice relationship. Thus, for example, once related compounds have been identified which bear a given lattice relationship to a new superconducting material, the related compounds can then be evaluated to see if they also exhibit superconductivity.

As still other examples, it can be important for the researcher to know whether two apparently different materials exhibiting the same property have the same or a derivative lattice relationship, or to identify an unknown phase by matching the unknown against all known lattice structures. Additionally, the researcher may wish to analyze structural lattice relationships within a large set of compounds, or between two sets of compounds.

Heretofore, analysis of lattice structures, both to determine intralattice relationships (e.g., lattice symmetries) and to determine interlattice relationships, has been difficult, cumbersome and subject to substantial error. For example, in the collection of crystallographic data, the experimentalist traditionally has relied on familiar or standard orientations to guide both the initial collection of data and evaluation thereof to define the lattice and the crystal symmetries. On a diffractometer, for example, a conventional unit cell, as defined by the magnitudes of the cell parameters, is determined and the assumed Laue symmetry is verified by taking specially oriented films or by checking the intensities of equivalent (h,k,l)'s listed for standard orientations. While there are many valid reasons for choosing conventional cells and orientations in the latter stages of experimental work, by choosing specific or familiar orientations in the initial stages, assumptions are made which influence what data are collected, and consequently, mistakes are more likely to be made.

In accordance with the present invention, a converse transformation matrix generation approach is used either i) to relate a lattice structure of one material to the lattice structure(s) of one or more other materials for determining interlattice relationships which allow materials to be identified and classified relative to other materials; or ii) to relate a lattice structure of a material to itself for determining lattice symmetry. The matrix approach is an extremely powerful, efficient and flexible analytical tool which is readily implemented and avoids the constraints and error inherent in the conventional approaches heretofore used. For example, the matrix approach is substantially more effective than prior approaches because it will maintain its selectivity in matching lattice structures despite the rather large experimental errors that are routinely associated with electron diffraction data. As another example, the determination of lattice symmetry using the matrix approach of the present invention does not require that the lattice and its symmetry be expressed with respect to a standard cell or a standard orientation. The properties of the lattice are reflected in any primitive cell because translation of the primitive unit cell generates the entire lattice. In accordance with the present invention, the symmetry matrices which transform the lattice into itself are generated, and are used to determine the metric symmetry and any pseudosymmetry, as well as the Laue symmetry, group-subgroup relationships, the nature and directions of symmetry axes, and conventional or standard cells. In addition, the determination of standard or conventional cells is greatly simplified. In contrast to other methods for determining standard cells, the matrix approach of the present invention permits working with symmetry directly in the form of matrices, and not with the magnitude of lattice parameters and their associated errors. Calculations are straightforward and a transformation matrix is found using linear algebra techniques.

Still further, the matrix approach of the present invention enables computer-based controllers for commercial diffractometers (x-ray, neutron and electron) to be implemented which fully automate the diffractometry process in a theoretically and experimentally correct and error-free manner. Unlike procedures currently used in diffractometry, errors in strategy are impossible with the matrix approach because at each step exactly the right data for control decisions are directly available in a clear, logical and concise format. Since the matrix approach is extremely reliable, its use will prevent errors in symmetry and structure determinations, which is widely recognized as a very serious current problem resulting in erroneous symmetry determinations in about five percent of the approximately 25,000 full structure determinations carried out annually.

The matrix approach of the present invention also enables electron diffractometry to be converted from a two dimensional technique that focuses primarily on d-spacings to a three dimensional technique similar to that employed in single crystal x-ray and neutron diffractometry. The ability to determine the cell structure and symmetry from data collected on extremely small samples and to identify the structure using computerized databases of known structures represents a new and comprehensive method to identify crystalline phases.

The matrix approach of the present invention thus represents a powerful new strategy for lattice structure analysis in which the emphasis is shifted from standard cells and standard orientations to matrices.