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Description of the F.C.C. Lattice Geometry Through a Four-Dimensional Hypercube

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Abstract

In an n-dimensional space, generally, n coordinates are used in a coordinate system. Using more than n coordinates, however, is sometimes more efficient in representing discrete spaces. This paper illustrates the application of using four coordinates to describe a three-dimensional face-centered cubic (f.c.c.) lattice. By the proposed method of description, all points in a f.c.c. lattice can be conveniently addressed by integer numbers. Many geometric computations in this discrete space are also much simplified in the new coordinate system.

Introduction

René Descartes, the 17th century French thinker and philosopher, is also remembered as an innovator in mathematics. His introduction of the concept of coordinate systems expanded the scope of geometry into analytical geometry. Scientists and engineers in all disciplines rarely do research without first choosing an appropriate coordinate system to represent the physical system involved. Mathematically, the purpose of a coordinate system is to address any point in the physical space concerned, be it continuous or discrete, with a convenient and unique set of indices called coordinates. In general, in an n-dimensional space, a set of n linearly independent coordinates are used.

The physical meaning of the values of the coordinates is distinctly defined in a particular coordinate system. A convenient definition is used in the familiar Cartesian system, as described in the following manner: in an n-dimensional space, we first select n mutually orthogonal $n-1$-dimensional subspaces as references for the n-dimensional Cartesian coordinate system. The coordinates of a point are then defined as an ordered series of the distances from that point to the n referential subspaces. The Euclidean distance is commonly applied in the above distance measurement. If a Cartesian coordinate system is used to describe a continuous space, all coordinates therein are real numbers. On the other hand, if the coordinates are all integers, the space being described must be discrete. For instance, the two-dimensional integer Cartesian coordinate system, commonly denoted as I^2, describes a planar square grid, while the three-dimensional integer Cartesian system, I^3, represents a spatial cubic lattice.

In theory, it is quite sufficient to use exactly n coordinates in an n-dimensional space. Using more than this number of coordinates only results in linear dependency among the coordinates. As a result, little theoretical study has been done on this seemingly redundant method of description. In practice, however, using more than n coordinates in an n-dimensional space sometimes results in a surprisingly efficient representation of a particular discrete space. Recent research (Her, 1993, 1995; Her & Yuan, 1994) shows, for example, such a coordinate system is used to effectively describe a two-dimensional hexagonal grid for computer graphics and vision. In this particular coordinate system, each point in a plane has three coordinates (x, y, z), instead of two, and they satisfy the following relation:

$$x + y + z = 0. \tag{1}$$

Fig. 1 illustrates part of the coordinate system in question. Since three coordinates are used, we have three corresponding referential subspaces (here they are lines) which are the $x = 0$, $y = 0$ and $z = 0$ axes, respectively. The coordinates (x, y, z) of a point mean that this point is on the xth line from the $x = 0$ axis, on the yth line from the $y = 0$ axis and on the zth line from the $z = 0$ axis. Note that in Fig. 1 the positive and negative sides of an axis are properly assigned. The three coordinate axes, intersecting one another at 60°, happen to be the axes of symmetry of a hexagonal grid. The aptly named *hexagonal coordinate system* is denoted as $*I^3$. The hexagonal grid, being the most densely packed arrangement in a plane, finds many applications in science and engineering (Mersereau, 1979). With the help of the hexagonal coordinate system $*I^3$, researchers can now easily perform many useful mathematical operations on the hexagonal grid, which were once considered prohibitively difficult (Bell, Holroyd & Mason, 1989; Her, 1995).

The purpose of this paper is to extend the concept as well as the advantages of the $*I^3$ coordinate system to a higher-dimensional space. By analogy, we now use four coordinates (x, y, z, w) to describe a point in a three-dimensional space. Similar to (1), we also assume that we have the following relationship among the coordinates:

$$x + y + z + w = 0. \tag{2}$$

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If only integer coordinates are used, this new coordinate system can duly be denoted as $*I^4$, and it will represent a particular lattice in the three-dimensional space. Since four coordinates are used, there must also exist four corresponding referential subspaces (now they are planes) in this coordinate system $*I^4$.

What kind of spatial lattice does $*I^4$ actually represent? Let us return and examine $*I^3$. From Fig. 1, we see that $*I^3$ in effect is a subspace in the three-dimensional Cartesian system I^3, and is the oblique plane mathematically defined by (1). The hexagonal tessellation of $*I^3$ results from the fact that this oblique plane slices a cube (the basic geometric feature of an I^3 lattice) into a regular hexagon. As shown in Fig. 1, half of the edges of the cube are cut in the middle. Owing to this relationship, $*I^3$ inherits many geometric properties from I^3 (Her, 1993; Her & Yuan, 1994). By the same reasoning, we realize that $*I^4$ is also a subspace in the four-dimensional Cartesian system I^4, and it is now a hyperplane represented by (2). The basic geometric feature of I^4 is a four-dimensional hypercube, and Fig. 2 shows such a hypercube (thin lines) projected onto a two-dimensional plane. What geometry do we get when a hypercube in I^4 is sliced by the hyperplane given by (2)? From the geometry of higher dimensions (Banchoff & Strauss, 1978), we learn that such an intersection is indeed a regular octahedron (as shown by the thick lines in Fig. 2), where half of the faces of the hypercube are cut diagonally by the hyperplane. Therefore, we see that $*I^4$ must represent an octahedral lattice in the three-dimensional space, and we can refer to $*I^4$ as the *octahedral coordinate system*.

An octahedron is a twelve-sided eight-faced three-dimensional geometric object with six vertices. If we put a lattice point at each of the six vertices in an octahedron (Fig. 3), we will have a basic octahedral lattice whose sides are exactly one unit long. In Fig. 3, we also show an octahedral lattice whose sides are two units long, and contains a total of 19 points. On examining this lattice closely, we realize that it is a face-centered cubic (f.c.c.) lattice. The f.c.c. lattice is one of the most closely packed lattice arrangements in three dimensions. In nature, the f.c.c. lattice is found in crystal structures of metals like aluminium, copper, silver and gold (Kalpakjian, 1989). In the following, we will use the f.c.c. lattice in Fig. 3 for further explanation.

As mentioned, there are four referential planes in the octahedral coordinate system $*I^4$. With reference to Fig. 3, we assign the center point O of the f.c.c. lattice as

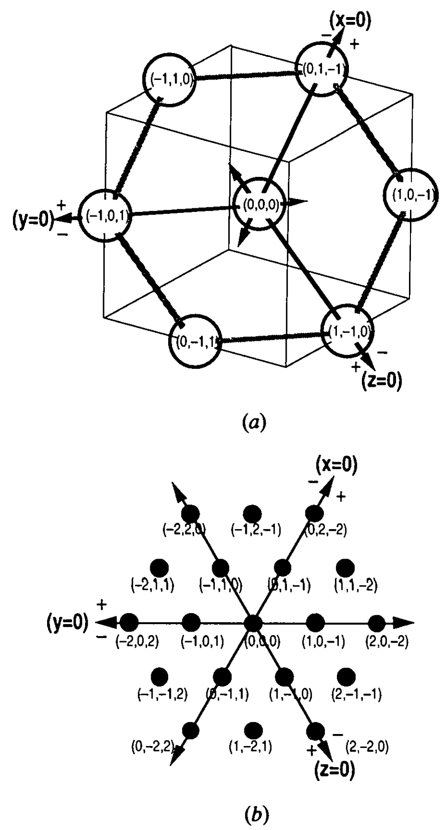

Fig. 1. A cube centered at the origin of I^3 is shown sliced by the $(x + y + z = 0)$ plane to form a hexagonal intersection (*a*), which is the basic feature of the hexagonal coordinate system $*I^3$ (*b*).

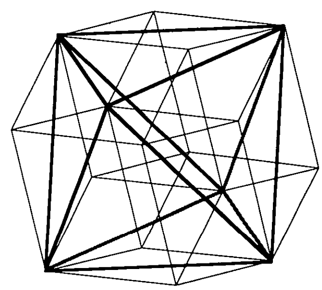

Fig. 2. A four-dimensional hypercube centered at the origin of I^4 and sliced by the $(x + y + z + w = 0)$ hyperplane. The intersection is a regular octahedron, which is the basic geometric feature of $*I^4$.

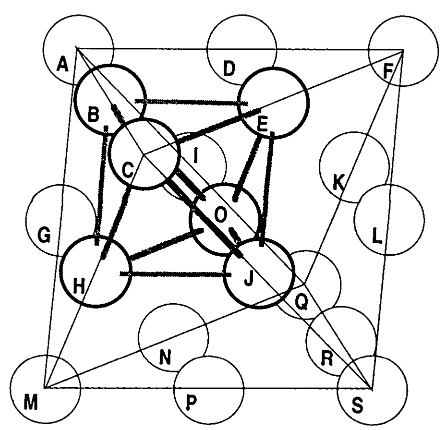

Fig. 3. An octahedral lattice whose side length is 1 unit (thick lines) contains only six lattice points, whereas an octahedral lattice whose side length is 2 units (thick lines plus thin lines) contains 19 lattice points.

the origin $(0, 0, 0, 0)$ of $*I^4$. The four referential planes are then represented by the four hexagons *GHJLKI*, *DEJPNI*, *BDKRPH*, and *BELRNG* containing the origin O. Each hexagon is parallel to two of the faces of the octahedron. Let us assume that hexagon *GHJLKI* is the $w = 0$ plane and w is positive above that plane. Comparing hexagon *GHJLKI* with the hexagon in Fig. 1, we can easily label the $*I^4$ coordinates of the lattice points on hexagon *GHJLKI*, as shown in Fig. 4. Since hexagon *DEJPNI* intersects the $w = 0$ plane at the $x = 0$ axis on that plane, it must correspond to the $x = 0$ reference plane in $*I^4$. Similarly, we see that hexagons *BDKRPH* and *BELRNG* are the $y = 0$ and $z = 0$ planes in $*I^4$, respectively. Now all lattice points in Fig. 4 can be labeled according to the assignment of these reference planes and their sign conventions. We encourage readers to add more f.c.c. lattice points to Fig. 4 and see what their $*I^4$ coordinates are.

In $*I^4$, the coordinates of a point (x, y, z, w) indicate that the point is on the xth plane from the $x = 0$ plane, on the yth plane from the $y = 0$ plane, on the zth plane from the $z = 0$ plane and on the wth plane from the $w = 0$ plane. A lattice point (x, y, z, w) has 12 immediate neighbors in $*I^4$ and their coordinates are:

$$\begin{aligned} &(x+1, y-1, z, w), \quad (x-1, y+1, z, w),\\ &(x+1, y, z-1, w), \quad (x-1, y, z+1, w),\\ &(x+1, y, z, w-1), \quad (x-1, y, z, w+1),\\ &(x, y+1, z-1, w), \quad (x, y-1, z+1, w),\\ &(x, y+1, z, w-1), \quad (x, y-1, z, w+1),\\ &(x, y, z+1, w-1), \quad (x, y, z-1, w+1). \end{aligned} \qquad (3)$$

Conventionally, the distance between any two immediate neighboring lattice points, for the sake of convenience, is defined as one unit. In $*I^4$, some spatial geometries that are difficult to describe in I^3 can now be easily represented. For example, consider the following formula:

$$|x| \le a, \quad |y| \le a, \quad |z| \le a, \quad |w| \le a. \qquad (4)$$

In I^4, this equation denotes a hypercube centered at the origin. However, in $*I^4$, as we can see from Fig. 4, it now represents a regular octahedral volume centered at the origin, and the length of its sides is precisely $2a$. In addition, it can also be shown that the following equation represents a regular tetrahedral volume, centered at the origin, and whose side length is equal to $4a$.

$$x \le a, \quad y \le a, \quad z \le a, \quad w \le a. \qquad (5)$$

Since the octahedral coordinate system $*I^4$ is, in fact, a subspace in the four-dimensional Cartesian system I^4, some geometrical computations in $*I^4$ must have very similar forms as those in I^4. For example, let the vertices of a regular tetrahedron in $*I^4$ have coordinates (x_i, y_i, z_i, w_i), $i = 1$–4. Then, by the mid-point law, the centroid of this tetrahedron must be located at $(1/4)\sum(x_i, y_i, z_i, w_i)$. Moreover, owing to analogy, the Euclidean distance between any two points (x_1, y_1, z_1, w_1) and (x_2, y_2, z_2, w_2) in I^4 is represented by the following formula:

$$[(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2 + (w_1 - w_2)^2]^{1/2}. \qquad (6)$$

From (3) and (6), we see that the distance between two neighboring $*I^4$ lattice points is $2^{1/2}$ units long in I^4. Knowing this scaling relationship, we can modify (6) so that it can readily be used to compute the distance between any two lattice points in $*I^4$. That is, the Euclidean distance in $*I^4$ is simply given as

$$\{[(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2 + (w_1 - w_2)^2]/2\}^{1/2}. \qquad (7)$$

It is clear that use of the integer octahedral coordinate system $*I^4$ and (7) facilitates greatly simplified distance measurements in a f.c.c. lattice. The distance function in (7) can also be used to define some spatial geometries in $*I^4$, *e.g.* spheres and ellipsoids. Finally, we note that there is a 48-fold symmetry in $*I^4$. This property is again very compatible to the description of a f.c.c. lattice.

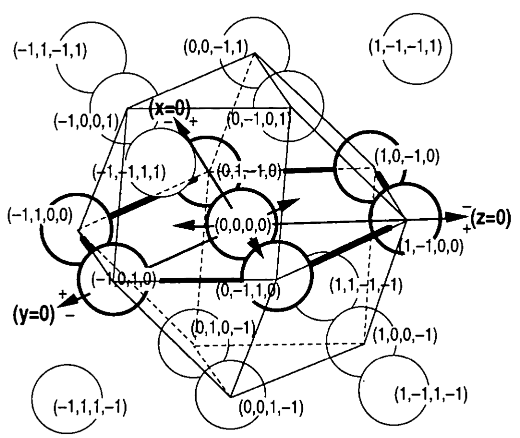

Fig. 4. All points in a f.c.c. lattice can be addressed by integer coordinates in $*I^4$. These coordinates, however, must satisfy the relationship $(x + y + z + w = 0)$.

Concluding remarks

This concludes our brief introduction on the use of the octahedral coordinate system $*I^4$, which is essentially a subspace in the four-dimensional Cartesian system I^4. Using $*I^4$, every point in a f.c.c. lattice can be addressed by integer coordinates and distance measurements among lattice points are very easy to calculate. A similar coordinate system, $*I^3$, used to describe a planar hexagonal grid, has been proved to be theoretically accurate and practically efficient as applied to many computer graphics and image-processing-related operations. The purpose of our study is to introduce these innovative coordinate systems to a wider audience, thus facilitating their use. In our opinion, the $*I^3$ and $*I^4$ coordinate systems will be useful in many areas of scientific and engineering endeavors.

The author thanks Mr Greg Ferrar for putting his *HyperCuber*2.0 program in the public domain. The drawing of Fig. 2 would have been difficult without this marvelous software. The author is also indebted to Mr Frederick J. Bailey Jr for his kind assistance in proofreading the manuscript.

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The Wavelength Dependence of Extinction in a Real Crystal: γ-ray Diffraction from NiF_2

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Dedicated to Professor W. Prandl on the occasion of his 60th birthday

Abstract

The wavelength dependence of extinction in an NiF_2 crystal of well known mosaicity has been examined by γ-radiation of wavelengths 0.0205, 0.0265, 0.0392 and 0.0603 Å. The results for seven strong low-order reflections, some of them symmetrically equivalent, are related to the extinction models of Becker & Coppens [*Acta Cryst.* (1975), A**31**, 417–425] and Sabine [*International Tables for Crystallography* (1992), Vol. C, pp. 530–533. Dordrecht: Kluwer]. In the considered wavelength region, the extinction-affected observed intensity is approximately a linear function of λ^2, and secondary extinction is found to be dominant. Allowance for pure secondary extinction according to the Becker & Coppens formalism yields both a satisfactory description of the wavelength dependence and mosaicities close to the directly observed ones. With the Sabine model, the influence of the mosaic distribution has to be excluded in order to describe the data properly. Hypothetical assumption of pure primary extinction, however, leads to nonrealistic mosaic-block sizes between 50 and 100 μm. This model is therefore not supported by experiment.

Introduction

Darwin's simple concept of the mosaic crystal and his energy-transport equations form the basis of standard extinction models, which all assume a clear-cut separation into two different extinction mechanisms. The intensity loss associated with coherent scattering in an individual perfect crystal block is termed primary extinction; the loss due to incoherent scattering from several different mosaic blocks is termed secondary extinction.

The theory of Zachariasen (1967) and its development by Becker & Coppens (1974, 1975) has been applied successfully in calculating structure factors close to the observed ones, even though it has some basic deficiencies. In particular, the Darwin equations involve intensities rather than amplitudes and thus the phase-dependent scattering in the case of primary extinction is not treated adequately (*e.g.* Lawrence, 1977).

Within the framework of intensity coupling, Sabine (1992) has proposed a theory in which primary and secondary extinction are treated in a unified way. His formulation, however, leads to an extinction correction factor that shows a substantially different dependence on physical quantities, especially on the wavelength, as compared to the previous theories. It has been included in Volume C of *International Tables for Crystallography* (Sabine, 1992), whereas descriptions of the widely adopted treatments of Zachariasen and Becker & Coppens are missing. It must be emphasized that the reliability of the wavelength variation of extinction corrections is of particular importance in white-beam diffraction techniques, which are used at synchrotron and pulsed spallation neutron sources.

γ-ray diffraction is well suited for an experimental test of different extinction models. Four wavelengths of