Mathematical structure

Mathematically, the points of the diamond cubic structure can be given coordinates as a subset of a three-dimensional integer lattice by using a cubic unit cell four units across. With these coordinates, the points of the structure have coordinates (x, y, z) satisfying the equations

$x = y = z \pmod 2$, and
$x + y + z = 0$ or $1 \pmod 4$.[5]

There are eight points (modulo 4) that satisfy these conditions:

(0,0,0), (0,2,2), (2,0,2), (2,2,0),
(3,3,3), (3,1,1), (1,3,1), (1,1,3)

All of the other points in the structure may be obtained by adding multiples of four to the x, y, and z coordinates of these eight points. Adjacent points in this structure are at distance $\sqrt{3}$ apart in the integer lattice; the edges of the diamond structure lie along the body diagonals of the integer grid cubes. This structure may be scaled to a cubical unit cell that is some number a of units across by multiplying all coordinates by $a/4$.

Returning to 3 dimensions, here is a very explicit description of the diamond cubic. It will be convenient to double the size of the diamond, so we can work with points all of whose coordinates are integers. So, start with a face-centered cubic consisting of points whose coordinates are even integers summing to a multiple of 4. It consists of these points:

$$(0,0,0),(2,2,0),(2,0,2),(0,2,2)$$

and all points obtained from these by adding multiples of 4 to any of the coordinates. To get the diamond cubic, we take this face-centered cubic together with another face-centered cubic that has been translated by the vector $(1,1,1)$

. That consists of these points:

$$(1,1,1),(3,3,1),(3,1,3),(1,3,3)$$

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