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Visualization of quasicrystal data

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A quasi-periodic crystal structure can be obtained by an irrational cut of the corresponding 5- or 6-dimensional periodic structure. This is done through mapping of 5D or 6D periodic space into orthogonal space by a transformation matrix. The first 3 dimensions of the orthogonal space are called as the parallel (or external or physical) space, in which atomic positions are described. The remaining dimensions are called as perpendicular (or internal or complementary) space. Up until now, visualization of quasicrystal structures has been done by exporting only the physical-space components of atomic positions in the Cartesian coordinate system and importing the data by conventional visualization software for crystal structures or molecules. However, such procedure leads to loss of any information about higher-dimensional symmetries, crystallographic sites etc., making it more difficult to correlate higher-dimensional space with 3D physical space. To overcome such limitation, an integrated visualization system VESTA [1, 2] has been extended to directly handle higher-dimensional data.

To deal with higher-dimensional data, dimension of vectors and matrices used in VESTA source codes are extended to accept arbitrary dimensions. In higher-dimensional space, an atom is represented by an “occupation domain”, which has specific size and shape along the complementary space. Quasicrystal structure data, i.e., generators of symmetry operations, atomic positions, and OD shapes, can be directly imported from the *.atm and *.pod files used by the QUASI07_08 package [3]. Furthermore, approximant structures can also be generated from the same higher-dimensional data by applying a phason strain matrix. On selection of an atom in the graphics area, its crystallographic information such as site name, fractional coordinates, coordinates in the orthogonal space, symmetry operation and translation applied to generate the atom from crystallographically independent site, etc., will be output on the text area. Visibility of each crystallographic site and its label can be turned on and off from a list of sites in the panel. Vector components such as magnetic moments and electronic polarization vectors are also dealt with higher-dimensional space. Symmetry operations can be applied to these vectors, and site symmetry constraints on their components are also checked automatically. If vector components violate the site symmetry constraint, the required constraint is output in the text area. Morphology of quasicrystals can also be visualized along with atomistic models, as shown in Fig. 1.

Figure 1. Atomic structure of the icosahedral Yb–Cd quasicrystal [4] overlayed on its hypothetical morphology, visualized by VESTA. Disordered atoms are not shown.


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