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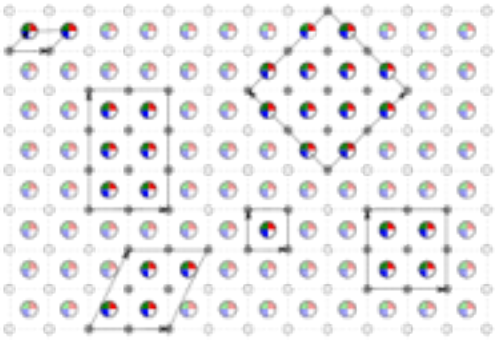
Supercell (crystal)

In solid-state physics and crystallography, a crystal structure is described by a unit cell. There are an infinite number of unit cells with different shapes and sizes which can describe the same crystal. Let's assume that a crystal structure is described by a unit cell **U**. The supercell **S** of unit cell **U** is a cell which describes the same crystal, but has larger volume than cell **U**. Many methods which use supercell perturbate it somehow to determine properties which cannot be determined by the initial cell. For example, during phonon calculations by the small displacement method, phonon frequencies in crystals are calculated using force values on slightly displaced atoms in the supercell. Another very important example of a supercell is the conventional cell of body-centered (bcc) or face-centered (fcc) cubic crystals.



An example of different supercell for 2D cubic crystal. Both diagonal and non-diagonal supercells presented.

Contents

Unit cell transformation

The basis vectors of unit cell **U** $(\vec{a},\vec{b},\vec{c})$ can be transformed to basis vectors of supercell **S** $(\vec{a}',\vec{b}',\vec{c}')$ by linear transformation[1]

$$\begin{pmatrix}\vec{a}' & \vec{b}' & \vec{c}'\end{pmatrix} = \begin{pmatrix}\vec{a} & \vec{b} & \vec{c}\end{pmatrix}\hat{P} = \begin{pmatrix}\vec{a} & \vec{b} & \vec{c}\end{pmatrix}\begin{pmatrix}P_{11} & P_{12} & P_{13}\\ P_{21} & P_{22} & P_{23}\\ P_{31} & P_{32} & P_{33}\end{pmatrix}$$

where $\hat{P}$ is a transformation matrix. All items P_{ij} should be integer numbers and $\det(\hat{P}) > 1$ (with $\det(\hat{P}) = 1$ the transformation preserve volume). For example, the matrix

$$P_{P\to I} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

transforms primitive cell to body centered. Another particular case of the transformation is a diagonal form ($P_{i\neq j} = 0$) of the matrix. This called diagonal supercell expansion and can be represented as repeating of the initial cell over crystallographic axes of initial cell.

Application

Supercells are also commonly used in computational models of crystal defects, in order to allow the use of periodic boundary conditions[2]. .

See also

- Crystal structure
- Bravais lattice
- Primitive cell
- Space group

References

1. Arnold, H. (2006). "Transformations of the coordinate system (unit-cell transformations)". **A**: 78–85. doi:10.1107/97809553602060000510 (https://doi.org/10.1107%2F97809553602060000510).
2. Okhotnikov, Kirill; Charpentier, Thibault; Cadars, Sylvian (2016). "Supercell program: a combinatorial structure-generation approach for the local-level modeling of atomic substitutions and partial occupancies in crystals". *Journal of Cheminformatics*. **8** (1). doi:10.1186/s13321-016-0129-3 (https://doi.org/10.1186%2Fs13321-016-0129-3). ISSN 1758-2946 (https://www.worldcat.org/issn/1758-2946).

External links

- IUCR online dictionary of crystallography (http://reference.iucr.org/dictionary/Main_Page)