

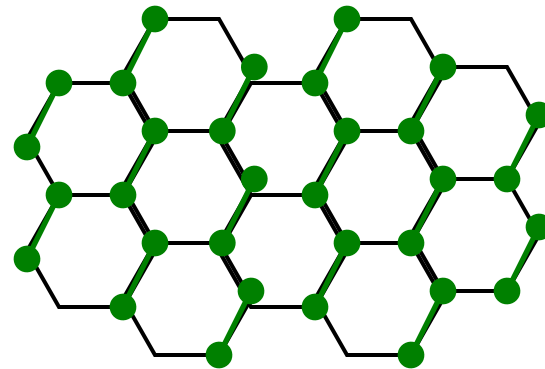
Building initial configuration. Ideal crystals (I)

Any crystalline solid can be defined in terms of *Bravais lattice*, which specifies the periodic array in which the repeated units of the crystal are arranged. Bravais lattice is defined by three *primitive vectors* $(\vec{a}, \vec{b}, \vec{c})$. Real crystal structure consists of identical copies of the same physical unit (group of atoms), called *basis*, located at all the points of a Bravais lattice.

Real crystalline structure = Bravais lattice with a basis.

The crystal structure is often discussed in terms of its *unit cell* – a basic building block of the crystal – the space limited by the parallelepiped defined by vectors $(\vec{a}, \vec{b}, \vec{c})$

Example: 2D honeycomb net is a triangular Bravais lattice with a two point basis.



Building initial configuration. Ideal crystals (II)

One can also describe a Bravais lattice as a lattice with a basis by choosing a non-primitive conventional unit cell. For example, although BCC and FCC are Bravais lattices (but not HCP – 3D analog of honeycomb) we can describe them as simple cubic Bravais lattices with primitive vectors $a\hat{x}, a\hat{y}, a\hat{z}$

and two-point basis for BCC: $\left(0, \frac{a}{2}(\hat{x} + \hat{y} + \hat{z}) \right)$

or a four-point basis for FCC: $\left(0, \frac{a}{2}(\hat{x} + \hat{y}), \frac{a}{2}(\hat{y} + \hat{z}), \frac{a}{2}(\hat{x} + \hat{z}) \right)$

These descriptions are implemented in MSE627-CG code.

Building initial configuration. Ideal crystals (III)

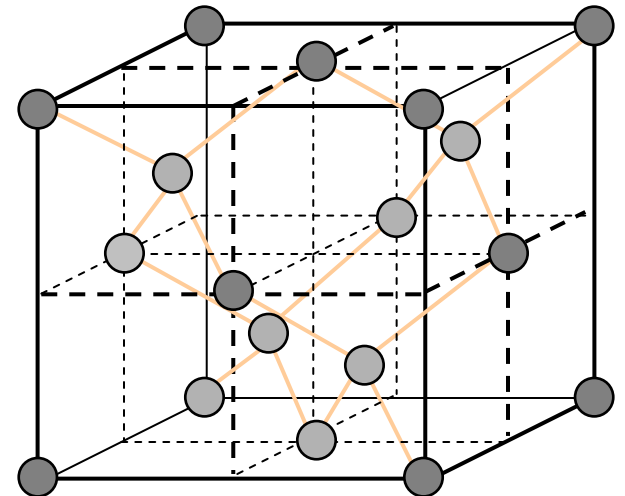
Diamond structure (C-d, Si, Ge, α -Sn)

Diamond lattice can be considered as two interpenetrating FCC Bravais lattices. Diamond lattice is not a Bravais lattice and can be described as FCC Bravais lattice with the two-point basis:

$$\left(0, \quad \frac{a}{4}(\hat{x} + \hat{y} + \hat{z}) \right)$$

But it is also possible to consider diamond lattice as a simple cubic Bravais lattice with 8-point basis

$$\left(0, \quad \frac{a}{2}(\hat{x}+\hat{y}), \quad \frac{a}{2}(\hat{y}+\hat{z}), \quad \frac{a}{2}(\hat{x}+\hat{z}), \quad \frac{a}{4}(\hat{x}+\hat{y}+\hat{z}), \quad \frac{a}{4}(3\hat{x}+3\hat{y}+\hat{z}), \quad \frac{a}{4}(\hat{x}+3\hat{y}+3\hat{z}), \quad \frac{a}{4}(3\hat{x}+\hat{y}+3\hat{z}) \right)$$



This latter description is implemented in MSE627-CG code.

Building initial configuration. Ideal crystals (IV)

Hexagonal close-packed (HCP) structure is also not a Bravais lattice, and can be considered as two interpenetrating simple hexagonal Bravais lattices.

Multi-component structures

Another class of crystalline structures for which we have to use a lattice with a basis are structures with more than one type of atoms, even if the atoms are located at the points of a Bravais lattice.

Sodium chloride structure (NaCl, KCl, MgO, CaO) consists of equal number of sodium and chlorine ions placed at alternate points of a simple cubic lattice. Can be described as FCC Bravais lattice with a basis consisting of two atoms.

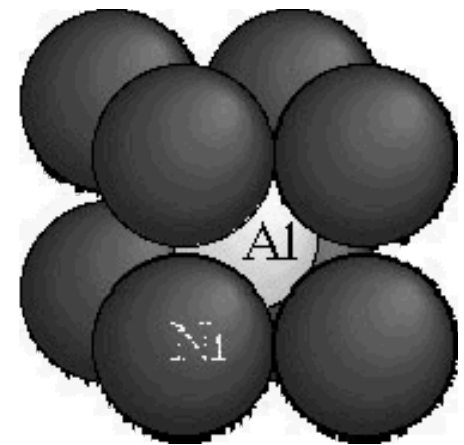
Cesium chloride structure (CsCl, CsBr) consists of equal number of cesium and chlorine ions placed at alternate points of a BCC lattice. Can be described as simple cubic Bravais lattice with a basis consisting of two atoms. Implemented in MSE627-CG code.

Building initial configuration. Ideal crystals (V)

Intermetallic alloys (Ni_3Al , Cu_3Au , Ni_3Mn)

Intermetallics are alloys composed of two or more elements, in which the unlike atoms have a strong affinity for each other. Interatomic bonding in intermetallics is still metallic in nature, but has an additional ionic character that is influenced by the difference in electronegativities between the constitutive elements. This attraction between dissimilar atoms forces the crystal to adopt a structure that accommodates these atomic bonding preferences. They have FCC structure which, however, is not a Bravais lattice. They can be described by simple cubic Bravais lattice with a four-point basis.

This description is implemented in MSE627-CG code.



Building initial configuration. Ideal crystals (VI)

Two-component systems with diamond structure (GaAs, SiC, ZnS)

These materials have their two components distributed on a diamond lattice so that each has four of the opposite type as nearest neighbors. This structure can be described as FCC Bravais lattice with the two-point basis or as a simple cubic Bravais lattice with 8-point basis.

The description is implemented in MSE627-CG code.

