

Abstract

The shape of crystals, quasicrystals and of microclusters depends on energetical optimality criteria. It is known since long, that the energetically optimal shapes are also "dense", with an intuitive idea of density. Since a couple of years it turns out, that besides the energy balance also the volume balance is optimal, i.e. besides the energy, minimal volume or maximal parametric density is an extremum property of crystals and quasicrystals.

In this thesis we consider the connection between these properties for microcluster. After introducing the basic concepts we investigate finite sphere-packings, which are subsets of the fcc-lattice or the hexagonal close packing (hcp). Thus we get a basic set of good packings. Thereby it is shown that octahedral packings, which are of minimal energy, are also dense.

We also state that deltahedral packings are energetically and geometrically optimal. Deltahedral packings do only exist for less than 13 spheres. For more than 12 spheres we determine packings which have minimal surface, like the deltahedra have. This set of packings contains a lot of optimal clusters (e.g. the so called Groemer-packings). We determine the optimal packings for other sets and shapes, like decahedral packings or bipyramidal packings. Packings with icosahedral shape are shown to be optimal if we allow ellipsoids as generalized spheres. Thereby we describe the difficulties of this approach.

All information about the packings is stored in a database which is available from the internet.