

The crystal structure - what information actually provides?

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A crystal consists of a set of molecules or ions ordered by periodic manner such that the overall free energy of the system is minimum. Such an arrangement is determined by the force action among the atoms which is related to size, shape, charge, dipole moments and hydrophobicity of individual molecules or ions. Due to the existence of a polymorphism and allotropism of crystalline materials it is obvious that despite these general principles, the arrangement of basic building particles in a crystalline solid will also depend on other factors. The shape of crystal is considerably affected by the conditions of its creation - and undoubtedly affect its inner crystal structure, too. These include temperature, pressure, concentrations of starting materials, the sequence in which the components are added, the crystallization method, the homogeneity of the environment and time. Sometimes a change of the arrangement of basic building particles in the crystal needed a big change some of these factors, sometimes it's a subtle change. As a rule, the lattice parameters obtained from single crystal and polycrystalline sample of the same substance may significantly vary in size (the differences often exceed more than ten times standard deviation). A possible explanation lies precisely in the different conditions of their crystallization. Important role to play here time and associated other factors. The process of creation of single crystals of suitable quality for structural analysis can be lengthy, whereas the formation of polycrystalline materials can be extremely fast. With such rapid processes you can assume numerous occurrence of inhomogeneities in the crystallization environment. The crystal structure arising microcrystalline substance will not reach the status of a global free energy minimum. If the energy barrier for example between polymorphs is small, there arise a mixture. A similar effect can also cause an isomorphic substitution of the atoms or ions in the crystal structure of the substance. In polycrystalline form there is possible to prepare the substance with any ratio of isomorphic atoms (ions), in the case of single crystal it is often practically impossible. The question then is whether there is a transition state of transformation from one polymorphic form to another, or there is always a mechanical combination thereof.

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