

Aspherical atom model - developing novel methods for crystal structure determination of partially disordered materials

Actual, extremely fast development of technology would not be possible without utilization of novel materials, unknown before. There is an urgent need to seek for connections between physical properties of those materials and their crystal structure. It has been shown that those properties are strongly correlated with atomic arrangement of atoms within the material. An important aspect of material's structure is to discover whatever atoms are organized in a periodic way and also if there are any deviations from the long-range structure on a local length-scale. Those local deviations can significantly change materials properties i.e. semi- or super-conductivity.

The primary tool for establishing material's crystal structure is X-Ray and neutron diffraction. All atoms (more precisely atom's electron distribution) within the material do scatter X-Ray radiation. The special distribution of scattered radiation gives us precise information on the atomic arrangement in the material. Based on this we can describe crystal structures in detail. A Spherical Atom Model, where all atoms are considered as being independent from each other, is used by the vast majority of the community. However, it does not take into account interatomic interactions and atomic chemical bonds. The existence of atomic bonds changes the electron distribution within the material and so its diffraction pattern. Therefore, an Aspherical Atom Model has been developed which includes these interatomic interactions and gives structural information more reliable.

The simple Spherical Atom Model is currently used by most crystallographers, and an Aspherical Atom Model can only be used when using single crystal diffraction experimental method. Within the current project we are aiming to extend the usability of the Aspherical Atom Model to other diffraction methods like powder diffraction, Pair Distribution Function or diffuse scattering.

As a main task of our project we are planning to implement an Aspherical Atom Model library called DISCaMB (currently under development at University of Warsaw) into Discus software package (developed at the Friedrich-Alexander-University Erlangen-Nuremberg, Germany).

The main planned outcome of the project is to develop new methods of materials investigations in the case of partially disordered structures which can provide much more precise information, reflection real atomic structure of the material.