Quasicrystals were discovered by Prof. Dan Shechtman in 1982 during standard measurements performed upon AlMn alloy. Simply speaking quasicrystals are crystalline structures with broken translational symmetry i.e. atoms are not arranged in periodic way. That discovery, awarded with Nobel Prize in Chemistry in 2011, changed scientific approach to the concept of order in crystals. Translation symmetry was no longer required for solid to be qualified as crystal.

Since the discovery scientific community struggles to find the best way to describe the structure of quasicrystal. Popular approaches i.e. higher-dimensional or cluster method are useful but quality of models is still unsatisfying. Due to complexity the knowledge about structure of quasicrystal especially conditions of quasicrystal formation is vague. Up to date knowledge allows to state that particular type of disorder in quasicrystals can be responsible for mysterious nature of aperiodic structures. That disorder is called phason.

Phason is the rearrangement of atoms in a way that the rest of the structure is unaffected. This rearrangement is noticeable in the diffraction measurements. Intensity of the peak measured with diffractometer strongly depends on the amount of phason disorder in the structure. Currently, this dependence is assumed to have the form of Debye-Waller factor in general form. Latest calculations show inadequacy in application of this factor. It was shown that it only works for: strong, high-intensity reflections or the structure with random arrangement of structure units. In other situations it fails.

The new approach completely changes the approach to phason disorder. If the distribution of atoms in quasicrystal is derived the phason flip can be detected due to its influence on the distribution, namely it is reshaped accordingly to the amount of flips in the structure. That methodology applied in theoretical simulation proved to improve structure model much better than application of Debye-Waller formula. Contrary to currently used correction the new one carries the information about probability of flip occurrence. It is valuable information which can give a glimpse on the structure formation process.

The project is focused on deriving new kind of phason disorder correction for decagonal and icosahedral quasicrystals and its application for selected alloys. New type of approach is expected to improve already solved models of quasicrystalline structures and bring completely new information, unreachable with the use of current theoretical tools.