Quasicrystals are crystalline structures with an aperiodic arrangement of atoms in space. It means that it is impossible to describe their atomic structure with a single group of atoms in the form of so-called elementary unit cell, duplicated and regularly arranged throughout the space. The correct description of the atomic structure of quasicrystals is, therefore, still a challenge, despite the passage of over 30 years since the discovery of this new family of materials. Methods known to describe classical crystals (periodic crystals) fail and new approaches must be applied. Recently, our team has developed a novel method of structure refinement based on the measured diffraction pattern. This method is fundamentally different from the classical Bragg or Laue approach and uses atomic probability distributions relative to a hypothetical reference network, referred to as the "average unit cell". Modeling the structure of quasicrystals boils down to modeling of this "average unit cell". This is a new approach and is not widely used, but has unique advantages that make it extremely interesting. The aim of the project is to apply this approach to the description of the structure of selected decagonal quasicrystals (with aperiodic arrangement of atoms in two-dimensional layers) and icosahedral (with aperiodic arrangement of atoms in three directions of space) - more precisely, creating models and refinement based on collected experimental data. The statistical method allows for effective consideration of all imperfections of the atomic structure. The main point here is to describe properly a blurring of the atomic positions around ideal positions due to thermal oscillations (phonons) and atomic shifts between such positions (phasons). An important aspect of our project is also the correct inclusion of the so-called scattering of a multiple radiation beam used for diffraction studies of crystalline samples. The aim of the project is to apply this theory to the cases of real structures and to examine the dependence of structural disorder on temperature. On this basis, we will answer the question, what mechanism makes aperiodic systems so complex. We will focus on the Al-Cu-Rh decagonal quasicrystal.

In the case of atomic structure analysis of three-dimensional (icosahedral) quasicrystals, we will answer the question about the role of the atomic cluster (grouping of atoms in the form of shell-like structures with the polyhedral shell shapes) in the formation of the structure. We have managed to grow unique crystal samples that will allow for high-quality structural studies. The very interesting is the relation of cluster-like structure with physical properties, like the recently discovered superconductivity in quasicrystals. The atomic structure models are crucial to predict, explain and describe properly physical properties. Our approach gives the only possible way to deliver a real-space model, which can be directly interpreted physically. We will focus on icosahedral Zn-Mg-{Hf,Tm} and AlZnMg systems with different cluster types. The last example is of particular interest, because of recently discovered superconductivity in quasicrystals. We will try to explain a role of Bergman-type clusters in superconductivity.

The project is of great cognitive importance in the field of structural research. It leads to the development of new methods of fitting the structure to the measured diffraction image. It allows you to search for a solution in a broader class of complex, both periodic and non-periodic structures. Some challenging questions corresponding to aperiodic systems, like phonons and phasons, multiple scattering, cluster ordering, and matching of the atomic structure model with physical properties will be answered as a result of our project.