DESCRIPTION FOR THE GENERAL PUBLIC (IN ENGLISH)

The main objective of the research project is to study the discontinuous reaction mechanism occurring in the solid state, with particular emphasis on discontinuous precipitation reaction involving grain boundary diffusion. The reaction of discontinuous precipitation allows to produce materials having a complex structure and good mechanical properties. The product formed during this reaction has a structure consisting of parallel plates of different chemical composition and spatial structure.

Reactions of discontinuous precipitation are a very interesting subject of research. So far researchers carried out a large number of experimental studies, which gave a lot of information, but did not explain the reaction mechanism. Therefore, computational studies are needed that will allow to understand the mechanism at the atomic level.

Molecular dynamics methods allow to create computer models that describe the motion of every atom in the material. The use of these computational methods in studies can help us understand the reaction mechanism of discontinuous precipitation and explain the experimental results accumulated in recent years.

Therefore, the proposed project focuses on in-depth knowledge and the description of discontinuous precipitation reactions occurring in the solid state, using the methods of atomistic simulations based on molecular dynamics. Obtaining an accurate description of discontinuous precipitation reaction will be useful in further stages of research on other reactions involving migration of grain boundary. The reaction of discontinuous precipitation leads to subsequent discontinuous reactions. Because of this, knowledge of the mechanism of this reaction, including the conditions and its starting point, is an important set of information that will allow to control microstructure of discontinuous precipitate. Ultimately, this will enable to understand and identify the individual stages of discontinuous precipitation reaction, and the accompanying physical phenomena related to energy, geometry, grain boundary diffusion and reaction front. Using a combination of different atomistic modeling techniques will allow to better understand the physical phenomena that determine growth rate and microstructure of reaction product formed discontinuous precipitation.