The most properties of engineering materials, e.g. physical, mechanical and thermal, depend directly on the microstructure, which in turn is a result of processes passing in the material during the forming and thermomechanical processing. The optimization of technological conditions of the process in view of final microstructure can be achieved using different modeling methods, for example with use the cellular automata (CA) and Lattice Boltzmann Method (LBM). The increasing of hardware capabilities makes possible use three-dimensional models that take into account much more parameters and approach the modeling to the real processes. These models require more memory and time for calculations, but more adequate modeling results can be obtained. The use of LBM and frontal cellular automata (FCA), which are a modification of the classical cellular automata (CA), allows to accelerate many times algorithmic calculations without loss of accuracy in the description of microstructural phenomena.

The main objective of the project are comprehensive experimental and theoretical studies of diffusion phase transformations in the solid state, occurring at low speed of cooling (transformation of austenite into ferrite and pearlite) and during the heating and soaking (transformation of the ferrite-pearlite structure to austenite, the alignment of carbon content in austenite and growth of austenite grains) in carbon steels (with a wide range of carbon content). Bearing in mind the diffusion character of the analyzed phase transformations, the model will take into account the issues of flow and heat transfer (generation or absorption of latent heat of transformation) and, first of all, diffusion.

The outcome of the project will be to develop a tool for adequate modeling and predicting the microstructure evolution in technological processes involving the aforementioned diffusion phase transformations. The development of such a model requires detailed experimental studies, which would precisely describe the phenomena occurring in the material and simulate them properly by using an innovative algorithm of three-dimensional frontal cellular automata, Lattice Boltzmann Method (LBM) and the latest software solutions with use of the high performance hybrid computing systems (CPU and GPU accelerators).

To achieve the main objective of this project, several tasks, which had a significant influence on the final model configuration and its capabilities, will be carried out:

- determination of the principal rules of phase transformations model based on the Frontal Cellular Automata (FCA) algorithm and the Lattice Boltzmann Method (LBM),
- dilatometric studies of the kinetics of phase transformations,
- microscopic examination of phase transformations,
- development of phase transformations model based on cellular automata,
- developing a model of flow, heat transfer and diffusion using the LBM method,
- parameters identification of the comprehensive model,
- modeling and verification of the phase transformations model,
- modeling of the technological process including: heating, soaking and cooling, and taking into account the phase transformations,
- analysis and verification of the modeling results.

Most of the developed models of microstructure evolution are two-dimensional and based on less complicated algorithms than the model proposed in the project. The developed model will take into account many factors which are neglected or treated too general in terms of the phase transformations. This includes diffusion phenomena and the kinetics of phase transformations. The model will be useful for solving these problems by allowing for faster calculations (CA + LBM), the use of any shape of grains, which is associated with the crystalline structure of materials and growth conditions, proper consideration of the diffusion process (LBM application) and allow to model correctly the kinetics of phase transformations.

The tasks which are planned in the project fit into the concept of the development of one of the strategic directions in science and economy, which is associated with materials engineering, foundry, metallurgical technologies and techniques. Digital Material Representation (DMR) is one of the most dynamically developing branches of materials science, including metal forming and heat treatment. The model could be interested for the scientists and technological engineers who are interested in complex consideration of the aforementioned diffusion phase transformations in carbon steels, in terms of the selection of appropriate technological parameters. The developed software can be a part of a system of the computer aided design (CAD) or engineering (CAE) for technological processes from the point of view of phase transformations. It could also be applied in the industry for a study of the real technological conditions and their influence on the final product. The project results, including the model, the algorithm and the software, can be used in education and as a virtual laboratory.