ABSTRACT FOR THE GENERAL PUBLIC

Project title:
Revealing the effect of diffusion on formation of the omega phase in metastable beta-Ti alloys: micromechanical insight from phase-field modelling

Modern aircrafts are among the most sophisticated machines. Their efficiency and reliability are based on decades of multidisciplinary research. The same applies to surgical fixation of fractures or surgical replacement of the hip or knee joint, which are among the greatest advances in medicine. In the mosaic of the required knowledge in these two completely distant fields, there is one shared piece. And this is the deep knowledge in materials science, in particular in the invention, design, and development of titanium-based alloys. Titanium alloys constitute metallic materials with a unique combination of properties: high-strength, reduced density, and excellent corrosion resistance. Most advanced alloys are used in the aerospace industry and medicine, others in architecture, sports goods, or even jewellery. Properties of these materials, and hence their applicability, strongly depend on the processing of these materials. In the development of metallic materials, we (after thousands of years) departed from trial-and-error experimenting to knowledge-based design and, of course, computer modelling.

This project focuses on modelling of the formation and evolution of peculiar nano-particles, known as omega phase particles, in titanium alloys. Quantitative predictions of evolution of these particles is critical for interrelating material processing and its performance. For this purpose, advanced and unique models will be developed, calibrated and validated. The models will be based on the phase-field method which is a powerful tool for modelling of phase transformations, such as that associated with the formation of the omega phase. The essence of the method is in introducing a diffuse-interface description of the interphase boundaries so that propagation of interfaces and evolution of micro-structure can be simulated on a fixed computational grid. Ultimately, model-based predictions will deepen the understanding of the mechanisms responsible for the formation of the omega phase.

The project will also join two research teams with different abilities, competencies, and equipment. One team, based in Warsaw, led by Prof. Stanisław Stupkiewicz, will be responsible mostly for developing phase-field models, based on long-term experience with this approach and with mechanics of materials in general. The other team, based in Prague, led by Dr. Karel Tůma, will focus both on the computer implementation of these models, including large-scale simulations, as well as on the experimental part of the project required for calibration and validation of the model. Experimental part will benefit from state-of-the-art characterization devices such as electron microscopes and x-ray diffractometers.