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Optimization of microstructure in heterogeneous materials - micromechanical and numerical modelling in non-linear regime

Micromechanical (multiscale) modelling is probably one of the most intensively developing modelling methodology in the scope of mechanics and material science. The goal of research in micromechanics is to estimate the macroscopic averaged properties of heterogeneous material (its *homogenization*) knowing the mechanical properties of the phases at the micro-level and morphological features and space distribution of components within the material representative volume. Estimated effective properties are then used in the design process of constructional elements fabricated with use of that material. The key component of the individual micromechanical models is a micro-macro transition scheme that enables to estimate the sensitivity of the macroscopic response to the changes in material microstructure and local properties. For example, the simplest scheme, often used in material science - *the mixture rule* assumes that all components of microstructure deform equally. In the frame of micromechanics the research effort is concentrated on proposing, by means of theoretical and numerical analyses, more refined description of the local strains and stresses redistribution in the material representative volume, and in this way more precise assessment of the response of such material under loading and/or due to temperature changes at the macro level. In view of their microstructure the heterogeneous media can be subdivided into those with periodic or random microstructure. In the first case a unit cell can be defined which by its multiplication in three directions fills the material volume. Materials with this type of microstructure are mainly synthetic ones like e.g. metamaterials - media with exceptional properties not met in nature. In the second case the microstructure can be characterized by a set of statistical distribution functions of same microstructural parameters: size and shape of components or their spatial distributions (packing) in the material volume. Among such materials there are natural (e.g. metal polycrystals) and synthetic (e.g. composites) materials. The materials with the random microstructure geometry are the subject of the present project.

Availability of reliable and efficient methods for predicting the effective properties of heterogeneous material is vital for their design process. With an increasing computer power and development of high resolution imaging techniques for microstructure characterization (e.g. computer tomography) the computational homogenization gains popularity in this field. By using the computed tomography (CT) scans a numerical model of the representative material volume is constructed. Accordingly, in order to specify local stress and strain fields, simulations are performed using the actual material microstructure. However, this homogenization technique for the heterogeneous media has its limitations. Due to a high computational cost, especially when the non-linear response regime is considered (large deformations, inelastic permanent strains) a reduced number of microstructure representative volumes can only be considered, so that the extensive parametric study of parameters, required for the optimal design process, is often burdensome or even impossible. In contrast to numerical analyses, analytical estimates of effective properties, being in the focus of this project, are an extremely efficient tool for designing and assessment of performance of newly-developed materials and the processing techniques applied.

The project results are of great significance for designing the multi-component and multi-functional materials (advanced metal and alloys, metal or polymer matrix composites dedicated to large strain regime and sensitive to strain rate, shape memory (SM) alloys and polymers in which the SM effect is related to the changes of composition and microstructure of the material under the external conditions as well as meta-materials) created for aviation, transport and electronic industries or for biomedical applications. Such materials are characterized by microstructures of complex geometry obtained by means of different thermomechanical treatment or, as in the case of meta-materials, by 3D printing technique. Such microstructures play a decisive role in establishment of desired performance of the material, i.e. high strength and stiffness combined with good thermal characteristics. The modelling tools developed in the project will contribute to the understanding of mechanisms that govern the observed relation between morphological features of microstructure at the local level and the material properties at the macro-scale. Understanding of such structure-property relationship is crucial for the material science and mechanics of materials communities. It is expected that the proposed models will give a possibility to design the material microstructure with a goal to obtain medium of desired properties and performance with respect to its future application.