DESCRIPTION FOR THE GENERAL PUBLIC

Practically all engineering materials contain interfaces such as interfaces separating the constituents in composite materials, grain boundaries in polycrystalline materials, phase boudaries accompanying phase transformations, and others. Importantly, the interfaces substantially influence the material behaviour, hence accurate modelling of the interfaces, including adequate representation of the interfaces in computational methods, is crucial for reliable modelling of the materials and, in particular, for gaining an improved understanding of the role of the interfaces. In some situations, for instance, during phase transformations, the interfaces may evolve, i.e. nucleate, propagate and annihilate, which gives rise to various interesting phenomena, but also makes the corresponding modelling more difficult.

The main goal of the present project is to develop new approaches and new computational strategies for the modelling of both non-propagating and propagating interfaces. A specific class of approaches will be considered in which the discretization introduced to numerically solve the problem does not match the geometry of the interfaces. This approach offers significant advantages, however, it also has a substantial disadvantage due to the additional approximation error introduced. The aim will thus be to reduce the related error, while keeping the advantages of the approach.

The improved computational schemes developed within the project will next be applied to solve selected problems of great interest in materials science. Three advanced materials, in which evolving interfaces play a particularly important role, have been selected for the study. The first material is the polycrystalline NiTi shape memory alloy (SMA). It has been observed experimentally that the martensitic transformation, which is the actual mechanism of inelastic deformation in SMAs, is often not homogeneous, but rather it proceeds through nucleation and propagation of macroscopic phase transformation fronts. The goal will be to study the structure of the macroscopic phase transformation fronts and to explain the mechanisms responsible for the inhomogeneous deformation. The second class of materials includes magnesium alloys in which plastic deformation involves an additional mechanism called deformation twinning. Twinning is a kind of displacive transformation that proceeds through nucleation and propagation of twinning planes. The physical mechanism of special interest is the reverse mode of twinning, in particular, the pseudo-reverse mode of twinning which has been recently demonstrated experimentally and which will be addressed in the present project. As the third material system, the layered structure of lithium-ion batteries has been selected. In this material, the phenomenon of interest in this project is the damage and fracture in the condition of mechanical abuse. This aspect is crucial for the safety of the batteries used for the propulsion energy storage in automotive applications, as even moderate mechanical impacts may lead to internal damage, short-circuit and fire hazard.