Mass transport processes at phase transformations occurring at moving boundaries of discontinuous precipitates- experiment vs. modelling

Grain boundary (GB) diffusion is one of the most important mechanism of mass transport. The GB diffusion plays a key role in many technological processes, being the base for production of advanced metallic and ceramic materials applied in electronics, energetics and nuclear industry. On the other hand, diffusion processes at GBs occur in a wide range during service. This can be, for example, liquation phenomenon in austenitic steels working at high temperatures, GB diffusion and migration in irradiated materials and processes in Fe-Zn coatings used in automotive industry for corrosion protection. Also the stimulus for electromigration and in a consequence to the degradation of electronic packages results from diffusion and migration. Therefore, the knowledge on GB diffusion parameters may guarantee the success in designing of these materials.

The most representative examples of phase transformations governed by GB diffusion is discontinuous precipitation (DP) and discontinuous dissolution (DD). They combine the occurrence of two phenomena, that is precipitation of a new phase and simultaneous movement of a high angle GB (reaction front-RF). In the past, these phase transformations were the subject of intensive studies which resulted in the statement that there is no difference in the rate of mass transport at the stationary and migrating GB. However, number of problems appearing in the course of DP and DD remained unsolved. The dramatic progress in capabilities of scientific instruments which took place during 10-15 last years, especially in the field of transmission and scanning electron microscopy, makes an unique chance to return to most of those unsolved problems of DP and DD. Moreover, application of atomistic simulations and a mesoscale model using nature of interatomic interactions will be helpful in discussion and analysis of the newly measured experimental data as well as give a deeper insight into the physical phenomena.

Therefore, the main scientific problem of the project is understanding the mechanism and kinetics of the mass transport during discontinuous precipitation and discontinuous dissolution combining experiment and atomistic simulations based on the three research hypotheses:

1. growing front of discontinuous precipitates must possess some intrinsic capability to react to balance the forces acting on it by some morphological modifications as the changes of the RF shape, re-nucleation, branching of precipitates, stop- and go or even backward migration of the RF. These morphological modifications are strictly related to the way of mass transport occurring at the RF.
2. the ‘history” stored in discontinuous precipitates determines the subsequent DD process, especially by the formation of “ghost images” of the former locations of the RF and precipitated phase. Again the way of mass transport is crucial in understanding instantaneous movement of the RF.
3. Mesoscale model combined with atomistic simulations will help in explaining the relationship between the mass transport and microstructural changes occurring along and across RF during DP and DD as well as for better visualization of physical phenomenon determining a limiting reaction transformation rate.

The results of the proposed project will create the scientific basis for the application of solid state phase transformations controlled by the diffusion at moving grain boundaries for the development of novel composite materials. In certain cases, the DP and DD reactions can be used for tailoring required properties of material like grain refinement or improvement of electric conductivity. The use of variety of atomistic methods will help to improve the description of physical phenomena, which influence the microstructure and chemistry of two-phase lamellar product.