Micromechanics of crystalline multi-component materials with non-standard deformation modes under non-monotonic loading conditions

Cyclic loading and the multiple strain path changes are common both during metal forming processes with large plastic strains involved, as well as during service conditions where limited strains are rather expected for a single loading cycle. Such processes lead to gradual material degradation due to accumulated inelastic deformation, modifying its stress-strain response and strength properties. These phenomena finally result in fatigue, an important factor defining structure durability.

Cutting-edge multicomponent materials, such us new magnesium or titanium alloys and refractory MAX phases, with high specific strength and stiffness, usually suffer from low ductility. Due to high plastic anisotropy, contrary to traditional metals or alloys deforming by dislocation motion, they often initiate non-standard deformation mechanisms such as **twinning/detwinning or kinking**. These straining modes are very sensitive to loading direction and produce **abrupt changes in material microstructure**, which accelerate the degradation process under non-monotonic loading. Materials offering high strength-to-weight ratios are ideal for aerospace, medical, and electronic applications, however, their unpredictable behaviour under cyclic loading is one of the reasons restricting their industrial use. Understanding how these materials' microstructures evolve under deformation could enhance their mechanical properties by modification of forming process or optimizing applied loads, and improve their reliability in service conditions. The availability of well-verified modelling approach, relevant for these materials and processes, is essential at the design and monitoring stage of structures. In this respect, physically-based, micromechanical models are especially useful.

The primary goal of this research is to develop **an advanced micromechanical model within the framework of crystal plasticity** to describe the relation between local deformation mechanisms and the material performance under complex, cyclic, and non-monotonic loading conditions. Within this methodology we estimate the macroscopic averaged (effective) properties of representative volume of heterogeneous material, i.e. we homogenize such medium, knowing how the mechanical properties of the phases at the micro-level and geometrical features of microstructure evolve along the non-monotonic deformation process. Contrary to the well-grounded of theories of crystal plasticity available in this respect for traditional alloys, the proposals and analyses addressing this problem for materials with non-standard deformation modes, highly sensitive to the loading direction, are in its infancy. The undertaken research aims to fill this gap.

The research comprises:

- **theoretical part** within which the existing crystal plasticity models are extended to account for non-standard straining mechanisms and tailored for non-monotonic loading processes, and then by means the micro-macro transition scheme allows to predict polycrystal behaviour,
- extension of **numerical procedures** including efficient implementation of the proposed single crystal and polycrystal models into finite element method which will allow, first, to verify correctness of the applied micro-macro transition scheme by enabling the analysis of representative polycrystalline samples, and next to simulate behaviour of prototype structural components,
- **experimental validation** of proposed models, encompassing mechanical testing combined with microstructural analyses of specially pre-designed samples of single crystals and polycrystals under cyclic and non-monotonic loading conditions.

This project aims to unravel microstructure-property relationship for materials with non-standard deformation mechanisms. By combining theoretical and numerical modelling with experimental validation, the research will provide tools for predicting the behaviour of innovative materials under real-world conditions. This will pave the way for designing materials and structures with improved strength, durability, and reliability for various high-performance applications.