Manufacturing and processing new materials with enhanced performance often require specific treatments involving different process temperatures, complex plastic deformation paths, or varying pressures. While these improvements offer benefits, they typically come at the cost of increased energy consumption, which is neither economically nor environmentally favourable. However, there are new processes available that can produce modern composite structures with enhanced properties by combining different conventional materials. One such process is the deposition of thin films, which allows for the combination of two materials with distinct properties.

Thin films are well-known for their ability to improve mechanical, thermal, strength, biocompatibility, and visual parameters. They find applications in various fields, such as protecting the surfaces of drills, jet engine components, artificial heart valves, or photovoltaic coatings. Understanding the behaviour of thin films under loading conditions is crucial, particularly in evaluating their strength. The complex columnar structure of thin films, resulting from the deposition process, often leads to uncontrolled delamination and cracking during operation, posing a significant challenge in providing reliable protection.

Analyzing the fracture mechanisms of thin films using experimental methods is complicated and time-consuming. Therefore, the project proposes the development of advanced numerical models based on the concept of digital material representation. These models will accurately capture the complex morphology of thin films and enable a detailed analysis of the local fracture. The project is divided into two parts, with the first part focusing on experimental studies to analyze the morphology of titanium nitride (TiN) thin films deposited using pulsed laser deposition (PLD) and physical vapour deposition (PVD) methods on different substrates such as titanium, steel, aluminium, and silicon. Scanning and transmission electron microscopes will be used for characterization purposes. The mechanical properties of the thin films and substrates will be tested using a picoindentation. Subsequently, the thin films will be cut and deformed under in-situ test conditions using a picoindenter integrated with a scanning electron microscope (SEM) to investigate the influence of film morphology on fracture initiation and propagation.

In the second part of the project, digital representations of thin films in 2D and 3D space will be created using image analysis algorithms, synthetic reconstruction models, and physics-based models of the deposition process. The experimental data and developed models will be used to identify critical parameters for crack initiation and propagation, which will then be verified through complex numerical simulations based on the finite element method. The proposed approach aims to bridge the gap between laboratory tests and simulations by developing accurate and representative numerical models to study the mechanisms of crack formation in thin films. This method has the potential to significantly reduce the time and cost associated with analyzing the strength of thin films, thereby opening up new possibilities for designing structures with desired properties. Integrated computational materials engineering will provide valuable insights for optimizing thin film design and improving their performance in various applications.