

1. Main target.

The main goal of the project is development and further application of the multi scale numerical model of nanoindentation test, connected with the digital material representation (DMR) approach for a detailed analysis of strength of the titanium (Ti) and titanium-nitride (TiN) nanolayers deposited with pulsed laser deposition (PLD) method.

2. Research topic.

Modern industry in order to fulfil the customer's needs have to design new types of materials. These innovative materials have to meet an economic, ecological and elevated in use properties requirements. Unfortunately well-known and widely used materials do not meet industry expectations. That is why materials scientists are trying to find another way to fulfil these high demands of manufacturers, contractors and traders, without exposing them to excessive costs. A worldwide idea for creating and using new kinds of materials is one of the goals of the European Framework Program of Research and Innovation (2014-2020) – „Horizon 2020“. Exploiting the cross sector potential of nanotechnologies and advanced materials to drive competitiveness and sustainability is one of the program challenges. The development of nanotechnologies and advanced materials with a view to their use in several different applications and economic sectors is a problem that matches this theme. The nano materials can boost the competitiveness of European industry and make contributions to a sustainable economy. This includes also contributions to European culture and creativity through novel materials. Experimental research is widely used, however it is related to excessive costs due to sophisticated equipment that is required at this scale level.

Thus, the main motivation of this project, is development of the multi scale numerical model capable to replicate material behavior during the nanoindentation test not only at the micro scale but also at nano scale level. The model will provide basic knowledge about material response as a result of local deformation.

To support the simulation a numerical model based on the idea of digital material representation (DMR) is proposed. DMR allows during numerical investigation to take into account morphology and mechanical properties of every single structural elements in deposited structure. It can be summarized that the DMR approach makes it possible to obtain a completely virtual description of the deformation process and provides better quality of numerical simulations for material scientists. Investigated DMR will be used to prepared multi scale nanoindentation models. Model at the micro scale will be upgraded by nanoscale model where nanostructure features will be taken into account (Figure 1). Digital models are often used in multi scale solutions that predict global material behaviour as well as can analyse microstructure changes during deformation in some critical/interesting locations, i.e. deformation response. Such an approach, which allows accurate replication of the material representation at the nano scale, is innovative and unique in the world, and its effect should bring the predicted behaviour of the material to its actual behaviour during deformation.

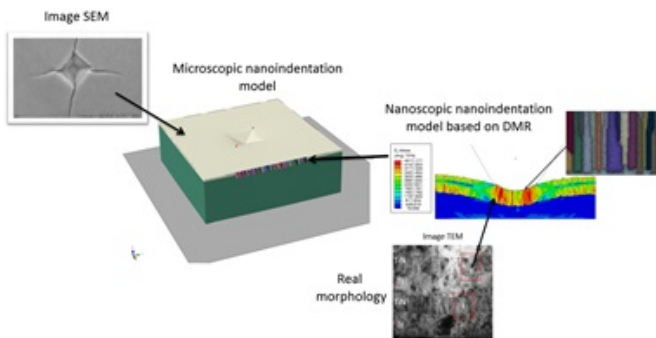


Figure 1 Schematically numerical procedure of nanoindentation tests.

Summarizing, the basic character of the proposed research is justified by its main goals that aim at broadening the knowledge on:

- processes occurring in nanomaterial during nanoindentation,
- digital representations of nanolayers,
- multi-scale modelling of materials using digital representations.

3. Basic research.

This work is divided into two stages: experimental and numerical (theoretically), respectively.

Experimentally:

The first stage is connected with experimental research, including the sample preparation with PLD process. Prepared samples will be subjected to nanoindentation tests. Information received after this stage will provide nanolayered material response during the local deformation. Obtained experimental data in the form of load-displacement curves will be an important parameter for numerical models validation. In this part microstructure analysis will be realized, to obtain images of microstructure for further generation of the DMR and to investigate local material behavior at the microstructure level prior and after deformation. These results will be also used for the model validation purposes.

Numerically(theoretically):

The second part, will focus on numerical research. During the part, the multi scale numerical model of the nanoindentation test will be created. Model will be composed of micro scale solution as well as digital material representation concept that can virtually take microstructure morphology into account. To obtain accurate digital material representations two approaches will be used: image processing of real microstructure photographs in 2D space and numerical methods based on discrete models e.g. Cellular Automata (CA), Monte Carlo (MC) in order to obtained 2D and 3D representations. The next step of the research, will

focus on connection of advantages provided by micro and nano scale models to establish concurrent multi scale solution. With these tools there will be a possibility to perform exact numerical analysis of the investigated material and support experimental research. General plan of research works is schematically presented in Figure 2.

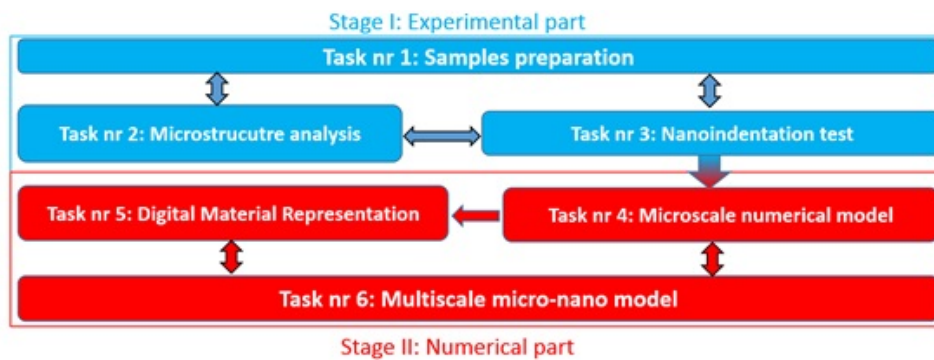


Figure 2 General idea of the project with classified main tasks.