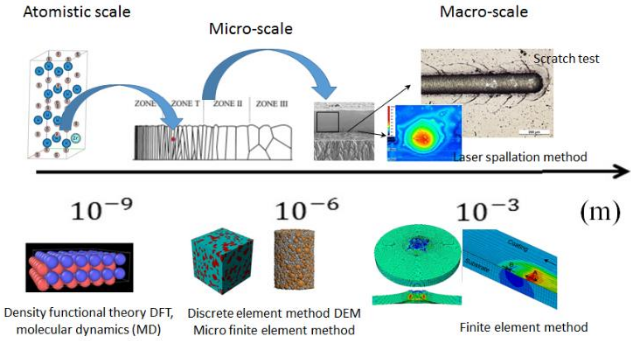
Hard and damage-resistant materials—their machining and application—have been at the centre of attention for a thousands of years. Unbreakable tools often saved lives and allowed for the progress of civilization. Today, resistant to damage in extreme conditions material research efforts are at their greatest ever level, thriving and attracting funding and industry attention worldwide. This is related to increasing the efficiency of the industry, but also to space travels planned in the near future. Currently, there is a trend of replacing expensive or difficult to synthesize materials such as diamond with their much cheaper counterparts. Very often, commercial materials are covered with thin layers, which significantly improve their reliability. The main problem of using super-hard and thermally resistant ceramics as protective layers is their brittleness and difficulties with adhesion to a much softer substrate. The last research reports on flexible hard ceramic coatings prepared by magnetron sputtering. Among them tungsten diborides represent a new class of coatings which are simultaneously super-hard, tough and resistant to cracking. Alloying of WB_x with transition metal like titanium, zirconium or tantalum leads to considerable improvement of mechanical and tribological properties compared to undopped borides. In this project these special mechanical properties of W-TM-B coatings will be obtained thanks to the use of High Power Impulse Magnetron Sputtering (HIPIMS) which provide the suitable balance of energy at deposited surface. Due to the fact that a material and its method of deposition are new, there is a lack of studies on mechanical properties of such coatings or they are insufficient.

In this project the comprehensive numerical and experimental analysis will allow us to investigate at various scales the mechanical properties and adhesion of novel ternary tungsten borides coatings deposited by HIPIMS.



Within the proposed project, development, implementation and validation of numerical models predicting mechanical properties and the deformation behaviour up to coatings damage will be performed for different scales: atomistic, microscopic and macroscopic one.

Fig 1: Overview of proposed multiscale model

The current state of knowledge points to the necessity of research towards a better understanding of relations between microstructure and material properties at different scales. Such a large number of material effects occurring at several scales during coatings loading cannot be described comprehensively with a one-scale approach. As base, density functional theory (DFT) and molecular dynamic (MD) will be used to obtain basic mechanical properties, also with taking into account of vacancies. The macroscopic mechanical properties of W-TM-B can arise also from material effects occurring at the microscopic scale also. Properties of borides depend on the type of structure ("V" shape or perpendicular to substrate grains), grain size (Hall–Petch effect), degree of amortization and distribution of the second boride phase (enhanced dislocation density) in the coating, what can be modelled with using of Discrete element method and/or micro-Finite element method. Further, the type of bonding determines ceramic coating features, and therefore the properties of the coating-substrate interface itself. The coating mechanical properties will be described starting from bond level (atomistic model) via interface separation (DEM) to fracture specimen in microscale (FEM) and failure resistance in macroscale. As a result the Laser spallation adhesion test (LST) will be modelled. The numerical models will be validated by the data obtained within the own multiscale experimental research. Experimental studies will consist of novel mechanical strength methods like: nanopilar compressing and cantilever bending, nanoidentation, and micro tensile tests. In addition, thermal resistance, wear resistance and other functional properties of the applied coatings will be tested experimentally.

The proposed interdisciplinary project focuses on (i) developing methods for efficient fabrication of superhard and flexible materials and their deposition on substrates as a coatings with high adhesion. The deposited coatings and coating-substrate interfaces will then be (ii) studied theoretically and experimentally in terms of their mechanical properties and the deformation behavior (up to the damage) in multiscale. The proposed theoretical models and experimental methods will also be (iii) used from the perspective of future applications of W-TM-B coatings, particularly in high temperature machining. Having in mind the possible industrial application, the crack resistance, flexibility and adhesion are one of the most crucial issues in the context of durability and long-term performance of super-hard coatings. Therefore, it is necessary to create a multi-scale model describing properties of deposited layers and the coating-substrate system also.