Topics of dissertations

Collaborating faculty:	**Materiálovotechnologická fakulta STU**
Academy year:	**2021/2022**
Study field:	**36 Engineering**
Study programme:	**Advanced materials and material design**
Length of study:	**4 years**

Topic 1: **Changes in the interface microstructure of copper-based composite materials with a carbon skeleton prepared by gas pressure infiltration**

Supervisor: **Ing. Jaroslav Kováčik, PhD.** (jaroslav.kovacik@savba.sk)

The aim of PhD work is to investigate the effect of technology control parameters; measure, and model properties of metal matrix composite materials prepared by the method of gas infiltration of molten metal into porous preforms. Composites with a copper based metal matrix reinforced with carbon porous skeleton will be investigated.
Volume changes due to the shrinkage during crystallization and shrinkage during cooling will also be evaluated. Therefore, it will be necessary to perform ab-initio calculations of the chemical composition of alloys suitable for infiltration, which would have the potential to meet the requirements of small volume changes. The selected systems will be then used to prepare composite materials by gas infiltration of molten metal into porous carbon porous skeleton. The technological parameters of the production process, especially temperature and time of infiltration, will be optimized. Also, the chemical composition of the metal matrix will vary, to which various elements will be added in very small amounts, depending on the desired type of carbide-forming reaction that ought to occur at the interface. The structure and composition of the interface will be investigated by means of electron and, if necessary, transmission electron microscopy. The influence of the created interface on the mechanical and thermophysical properties of the composite will be also investigated.

Topic 2: **Development of a new biomedical composite with TNTZ matrix and biodegradable component (Zn, Mg, Ca) with low modulus of elasticity and increased surface bioactivity**

Supervisor: **Martin Balog, PhD.** (martin.balog@savba.sk)
Co-supervisor: Ing. Peter Krížik, PhD.

The aim of the doctoral thesis is the development of a new bulk composite material with Ti (TNTZ) matrix and biodegradable component (Zn, Mg, Ca) with an extremely low modulus of elasticity for the application of permanent biomedical implants subjected to intense and cyclic loading. The developed material aims to minimize the basic shortcomings of current Ti implants, namely mechanical incompatibility (so-called stress-shielding effect) and insufficient surface bioactivity. During the interdisciplinary work the doctoral student will be responsible for: i) fabrication and optimization of composite preparation technologies of powder metallurgy and hydrostatic extrusion, ii) complex microstructural characterisation, iii) optimization of TNTZ matrix chemistry and determination of biodegradable component influencing mechanical and fatigue properties,

iv) determination of corrosion resistance and rate of degradation of the biodegradable component in simulated body fluids, v) in-vitro cell culture response studies, i.e., viability, proliferation, DNA degradation, oxidative stress of the optimized composite materials. The doctoral student will be required for both experimental and analytical type of research. The doctoral student will have to handle various technologies of powder metallurgy, will use the methods of thermal analysis (TGA, DSC) and electron microscopy (SEM, TEM), spectrometric methods (EBSD, EDS), X-ray diffraction (XRD), mechanical (tensile tests, DMA) and fatigue tests, at collaborative bases he/she will participate on in-vitro cell culture biological response (MTT) assays. The doctoral thesis will be supported by an applied research project and the student will work closely with the BMC SAS and other foreign institutions. A previous experience related to a given type of materials research, fluent and active knowledge of the English language, the ability to work in a dynamic team and independence are required.

Topic 3: **Influence of hydrogen on deformation behavior and fracture of complex concentrated alloys**

Supervisor: **Ing. Juraj Lapin, DrSc.** (juraj.lapin@savba.sk)

Hydrogen is a key priority of the European strategy for clean energy and metallic materials are a key pillar of expected technical solutions and innovations in its production, storage, distribution and end-use. PhD thesis will be focused on investigating the influence of hydrogen on the deformation behaviour and fracture of Co-Cr-Fe-Ni type complex concentrated alloys (CCA). The PhD student will participate in the metallurgical preparation of alloys with the required chemical composition, characterization of their microstructure and investigation of the effect of hydrogen on their deformation behaviour at room and low temperatures. He/she will investigate the deformation behaviour of CCA during tensile, compressive, fracture toughness and impact fracture toughness tests. Using the finite element method and the ANSYS program, he/she will simulate the deformation behaviour of the investigated CCAs, determine the critical local stresses and critical local deformations needed for crack initiation and propagation. Numerical calculations will be verified experimentally. The candidate is required to have experimental skills, knowledge of applied mechanics, basic knowledge of materials science, knowledge of mechanical testing of materials, knowledge of numerical calculation methods as well as a good knowledge of English.

Topic 4: **The concept of diboride superlattices with improved fracture toughness**

Supervisor: **doc. Ing. Marián Mikula, PhD.** (marian.mikula@savba.sk)

The dissertation deals with the improvement of fracture toughness in inherently hard and brittle diboride coatings prepared by PVD techniques. These ceramic coatings based on transition metal diborides (TMB_2), in particular TiB_2, ZrB_2 and TaB_2, are generally characterized by a nanocomposite character, where TMB2 nanofilaments are surrounded by a thin, amorphous boron-tissue phase. Such a nanostructure leads to excellent mechanical properties, in particular of extremely high hardness H> 40 GPa. Unfortunately, diborides are also characterized by low fracture toughness, which is defined as the ability of a material to resist the initiation of cracks that further propagate and cause fracture. A very promising concept for improving fracture toughness seems to be the formation of superlattices during growth of the films, which has proven successful in transition metal nitride (TMNs)-based coatings. Superlattices are formed by very thin diboride layers, (e.g. TiB_2-TaB_2) with a thickness of several nanometers, which periodically grow on each other. Different lattice parameters and shear moduli cause a weakening of crack propagation and their deflection at the interface between the layers, which is reflected in increased fracture toughness.

For the preparation of selected hard coatings, modern approaches in physical vapor deposition will be used, especially magnetron sputtering. In addition to measuring the mechanical properties of coatings by nanoindentation techniques, their other important properties related to the mechanical behavior of hard diborides will be investigated using several analytical methods: thermal stability of formed nanostructures, their decomposition mechanisms, formation of metastable and stable phases, oxidation resistance by means of scanning electron microscope (SEM),energy-dispersive X-ray spectroscopy (EDS), wave-dispersive X-ray spectroscopy (WDS), ultraviolet photoelectron spectroscopy (UPS), X-ray photoelectron spectroscopy (XPS), X-ray diffraction analysis (XRD), transmission electron microscopy (TEM) and others. The evaluation of fracture toughness will be performed using a picoindenter in SEM on cantilevers prepared by focused ion beam (FIB).
The dissertation will also use ab initio calculations to predict and better understand the mechanical behavior of the layers and interpret the results.

References

1. M. Mikula, S. Uzon, T. Hudec, B. Grančič, M. Truchlý, T. Roch, P. Švec jr. , L. Satrapinskyy, M. Čaplovičová, G. Greczynski, I. Petrov, M. Odén , P. Kúš, D. G. Sangiovanni: Thermally induced structural evolution and age-hardening of polycrystalline $V_{1-x}Mo_xN$ (x~0.4) thin films, Surface and Coatings Technology, 405, 126723 (2021)
2. N. Koutná, A. Brenner, D. Holec, P. H. Mayrhofer: High-throughput first-principles search for ceramic superlattices with improved ductility and fracture resistance, Acta Materialia 206, 116615, (2021)
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4. M. Mikula, B. Grančič, P. Švec jr., T. Roch, M. Truchlý, O. Kohuľák, L. Satrapinskyy, T. Fiantok, V. Izai, M. Haršáni, Ľ. Orovčík, P. Kúš: Thermally-induced structure evolution in ternary $Ti_{1-x}Y_xB_{2+\Delta}$ films, Scripta Materialia (2019) 91-95