## Reg. No: 2021/43/D/ST8/03183; Principal Investigator: dr in . Jakub Kawałko

Properties of many materials are determined by their internal microscopic structure or microstructure – a set of features such as the size and shape of grains – small crystals which are the building blocks of most of metallic and ceramic materials. Atoms in a single grain, like in a crystal are arranged in a three dimensional periodic pattern – crystal lattice. Because of this perfect periodic arrangement, atoms in crystal lattice are relatively stable – they are resistant to deformation and chemical attacks or corrosion. However in a typical polycrystalline material single grains are really small, and in one cubic centimeter there could be many millions of them. Between the grains – in the **grain boundaries** there are areas where atoms are not in their perfect position as they cannot fit to crystal lattice positions of both of the neighbor grains at the same time. Increasing the number of those 'random' grain boundaries can improve mechanical properties – **boundaries** act as barriers for dislocations – crystal lattice defects by movement of which the grains get deformed. But increasing number of grain boundaries also increases number of 'unstable' atoms which aren't in their ideal crystal lattice positions. This can lead to **grain boundary sliding (GBS)** – the mechanism of creep in increased temperatures – deformation of material under lower stress than its typical strength, or decreased corrosion resistance as atoms in grain boundaries are less resistant to chemical attack.

Fortunately it is possible to arrange grains in a polycrystal to mitigate those negative effects of grain boundaries. In the certain 'special' grain orientation relationships, called **coincidence site lattice (CSL) misorientations**, a fraction of ideal atom positions from one grain can *coincide* (overlap) with atoms in the other grain. The more *overlap* there is between two grains, the more *stable* the grain boundary is. The types and quantities of grain boundaries in the metallic material can be affected and controlled through various ways such as special mechanic and thermal treatments. Those treatments can generally be described as **grain boundary engineering (GBE)** – and applied to increase or control certain grain boundary related properties of a material such as creep or corrosion resistance.

In this project we decided to apply the concepts of the **grain boundary engineering** to zinc alloys that have the potential to be applied in bio-resorbable temporary implants, such as cardiac stents or bone screws. The corrosion properties of those zinc alloys are ideal for cardiac stents, however their mechanical properties should be improved before they can be safely applied. Zinc melting temperature is really low for a metal – 419.5 °C, therefore it is quite prone to creep at the temperature inside human body.

In this project we will be investigating how the different types of grain boundaries affect the mechanical properties of zinc alloys, and what types of processing can increase fractions of CSL grain boundaries in those materials. To investigate the grain boundary types and properties we will be using advanced electron microscopy techniques and micromechanical testing equipment. To analyze grain boundaries we will be using electron back-scattered diffraction (EBSD) in scanning electron microscope (SEM) to create maps of grain orientations, which will allow the calculation of grain boundary misorientations. Chemical analysis of grain boundaries in terms of alloying atom concentration and secondary phases precipitates will be also investigated using high mas resolution time-of-flight secondary ion mas spectroscopy (ToF-SIMS). This information will then be correlated with macroscopic properties: tensile strength and creep resistance. Combined with the EBSD we also will be using a tensile stage inside SEM in order to observe the deformation mechanisms and GBS in-situ. In addition we will be using a focused ion beam (FIB) system inside SEM to prepare microscopic specimens containing either single grain or two grains and one grain boundary. Next, by using precise nano-indenter in SEM we will be able to test mechanical properties and simultaneously observe the deformation of single grains and single grain boundaries. This will allow us to describe the relationships between grain boundary type (special or random) and their deformation behavior.

The results of this project will provide new insights into the relationships between grain boundary microstructure and properties of zinc alloys, and will be important step in the development of zinc based bio-resorbable implants.