DESCRIPTION FOR THE GENERAL PUBLIC

Intense research in green technologies is focusing on reducing energy consumption in all transport sectors, providing incentives for designing new light and strong materials. Taking into account these two parameters, it is clear that hexagonal metals like Ti, which has one of the highest strength-to-density ratios, are potentially prime elements when considering new constructional materials. One of the main problems limiting extensive usage of hexagonal metals is confined ductility of their alloys, essentially increasing production costs. As a consequence, much effort has gone into developing plastic deformation theory and practical methods that allow one to predict the mechanical behaviour of materials [1].

The mechanisms determining mechanical properties of metals are dislocations emission and motion supported by twinning (plastic deformation modes, active at room temperature). Previous investigations revealed that, owing to cross slip facility, screw dislocations act as a dominant deformation mode of Ti [2]. However, the activity of line defects (dislocations) depends substantially on the grain size and alloying elements type or their concentration. While the microstructure can be controlled by plastic or heat treatment, changes in chemical composition require complex knowledge of the influence of each element on line defects energy and mobility. Due to the reduced symmetry of hexagonal crystals and the numerous possible modes of dislocation motion, these relationships remain unknown. An additional motivation to clarify the above dependencies comes from the new, outstanding effects observed recently in single phase hexagonal alloys, such as unusual ductility improvement in Mg+Y systems [3], radical strength enhancement linked with well-balanced plasticity of α-Ti+O solutions [4] and the special, both strength and ductility improvement reported in α-Ti+In alloys [5]. The sophisticated character of solute-dislocation interactions can be described by materials modelling methods, which include quantum mechanics tools needed to reproduce correct dislocation core structure, atomic bonds type, their distribution and energies. The latest scientific reports on such computations reveal the existence of previously unknown atomic scale phenomena like split of slip modes [6], polymorphism of screw dislocation cores (numerous core geometries able to exist simultaneously at finite temperatures) [2] and line defect reconfiguration occurring in the alloy element vicinity [7]. These novel effects were not considered in the current solution strengthening theories, which further complicates hexagonal alloys design methodology.

Accordingly, the overall objective of the project is to identify the solution strengthening mechanisms of α-Ti alloys through systematic analysis of the impact of alloying elements on the behaviour (geometry, energy and motion) of screw dislocations, which mostly determines the mechanical properties of hexagonal alloys. To this end, comprehensive atomic scale, *ab initio* calculations will be performed to describe physically basic rules of solute and line defect interactions and other, structural factors influencing geometry, stability and motion of screw dislocations. The scope of the project will be further enriched by experimental works oriented on empirical validation of the method and elaborated theory. Selected developed alloys will be fabricated in the experimental part of the proposed project using the arc melting method and subjected to mechanical properties, microstructure, phase and chemical composition investigations (verification of the chemical homogeneity and single phase composition of fabricated materials). Comparison of the theoretical (predicted strengthening level) and experimental (final mechanical properties) studies will determine which strengthening mechanism plays a crucial role in the case of α-Ti alloys.

The results of the planned research are fundamental to understanding the recently observed superior properties of hexagonal materials (great strength and ductility) and adopting them in a controlled manner to new alloys. The gathered knowledge will have a broad impact on the field of atomistic modelling of plasticity, where screw dislocation modelling is the current challenge [1,2,7]. It will also mark a step forward in conscious design of novel, lightweight hexagonal alloys with expected mechanical properties. Finally, novel light metallic materials are commonly found in vehicles, wind turbines, sport equipment, aircraft industry, biomedical devices and other applications. Development of this material group has a direct influence on living standards and reductions in the emission of pollutants.

References:

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