DESCRIPTION FOR THE GENERAL PUBLIC

Increasing emission of greenhouse gases and continuous climate change is currently of prime interest and provokes radical boost of green technologies focused on reduction of energy consumption. Such approach can be met in all types of transport sectors, especially in automotive and aircraft branch where design of new, fuel efficient engines and lightweight constructions are crucial. Regarding to the latter issue, available reports indicate 6 - 8 % decrease in fuel consumption for a 10 % weight reduction of cars and trucks [1] as well as 5.1 % improvement in fuel economy of hybrid vehicles and 13.7 % increase in maximum range of electric cars [1]. Such limitation of fuel use leads to suppression of the global emission of CO_2 by few tens of million tons per year [2]. The above numbers illustrate the large pressure oriented on design of the new lightweight structural materials, attractive also for other industrial branches.

Among all lightweight metals, Ti is the only one belonging to the transition metals (TM) group which due to presence of *d*-type electrons posses mixed, metallic and covalent character of bonds. Number of these electrons influences directly on the structure and properties of TM, and act as useful parameter for material design process. The above relation is also true for elastic anisotropy which is typical for all crystalline materials because of their non-identical, atomic-scale periodicity at different crystallographic directions. Available experiments, demonstrate however, that fully elastically isotropic TM alloys are possible to occur at specific average number of valence electrons [3]. Required, electronic conditions to reach elastic isotropy can be achieved in body-centered cubic (β) Ti-V alloys [3] and according to the newest thermodynamic data [4] in lightweight and low-cost ternary compositions, *i.e.* β-Ti-Fe-Cr systems (total Fe and Cr content below 30 at%). Such materials should exhibit great mechanical properties due to perfectly homogeneous response to elastic load (lack of internal stress concentration). On the other hand, the influence of elastic anisotropy on ductility is poorly understood as TM exhibit also plastic deformation anisotropy arising from specific configuration of dislocation (line defect which glide control plasticity of metals) cores. The elastic and plastic anisotropy is essential for all structural materials since it determines their fatigue behavior and ductility. These properties are especially important for lightweight metals like Ti, suffering due to low cold workability, which increases production cost and limits application range.

Accordingly, the overall objective of the project is to reveal the influence of unique, elastic isotropy of the new group of Ti-based alloys on their mechanical properties in the regime of elastic load like fatigue limit and those controlled by plastic deformation *i.e.* yield and tensile strength, work hardening and elongation to failure. The foreseen properties of these systems are highly desirable, especially for applications were high strength-to-density ratio plays the major role. Nevertheless, due to limited knowledge about discussed alloys there are fundamental questions needed to be solved. Presented issues are related to the basic atomic scale phenomena which are nowadays intensively explored using the quantum-mechanical modeling methods [5–12]. Such approach is also planned in this project *i.e. ab initio* design of the new elastically isotropic ternary Ti alloys and investigation of elastic/plastic anisotropy expanded by fabrication and experimental measurements of developed systems. The gathered data will be highly useful for further development and conscious design of the new lightweight and affordable Ti-based materials with attractive properties.

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