Project 6.4 Elastically isotropic and metastable body-centered cubic titanium alloys -First principles and empirical investigation

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Background:

The main driving force of the overall project is to relate elastic anisotropy with plastic deformation of BCC systems based on the new, perfectly elastically isotropic Ti alloys group. These systems have a unique ability to undergo fully homogeneous deformation instead of heterogeneous strain/stress distribution which favors crack nucleation and limits ductility as in typical polycrystalline alloys. Such features, i.e. lack of elastic mismatch between particular grains and the resultant uniform dislocation density inside them, is highly desirable from the processing and material reliability point of view. The impact of the elastic anisotropy on the plastic deformation is poorly understood as both hexagonal close-packed (HCP) and BCC TM exhibit also plastic anisotropy linked with polymorphism of dislocation cores and their glide trajectory, intensively investigated within last years. The discussed elastic and plastic anisotropy is essential for all constructional materials as it determines fatigue behavior and ductility. These properties are especially important for lightweight metals like Mg or Ti (both with HCP structure) suffering due to low cold workability, which increases production cost and limits application range. Moreover, mechanical properties of Ti alloys can be successfully tuned not only by e/a but also through careful adjustment of chemical composition including interstitial elements like oxygen or simple metals (SM) i.e. Al, Sn, etc. These elements have significant impact on dislocation glide and in general, on activity of particular deformation modes of HCP Ti. Available literature does not provide any data about such relation in Ti alloys with high e/a which generates some crucial questions needing further explanation.

Aim:

The overall objective of the project is to reveal the influence of 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. In addition to general objective, three special goals have been set: (i) bottom-up (ab initio) design of the low-cost, elastically isotropic body-centered cubic (EIBCC) Ti alloys, (ii) description of the influence of different types of solutes (substitutional transition/simple metals) on activity of the particular deformation modes of EIBCC crystals and (iii) experimental determination of mechanical properties of the EIBCC alloys based on tensile and fatigue tests.

Requirements:

- experience in DFT simulations and data analysis
- Bachelor or Master degree, or relevant working experience
- proficiency in English