Abstract

The thesis introduces the application of *ab initio* methods in the field of elasticity theory, enabling the determination of elastic and other material properties while indicating the limits of the method's accuracy for specific transition metals. It includes a discussion of exchange–correlation functionals beyond PBE (Perdew, Burke and Ernzerhof) that exhibit strong agreement with experimental measurements. Furthermore, it presents and describes physical phenomena observed in crystalline structures under applied shear stress—topics that have been the subject of intensive research in materials physics in recent years.

The main objective of the work is to investigate grain-scale elastic isotropy in titanium alloys. Elastic isotropy is a highly unusual property in crystalline structures, and its origin is quantum in nature, stemming from the distribution of atomic orbitals; it cannot be explained solely on the basis of electrostatics. The thesis presents theoretical results based on density-functional theory and statistical methods that make it possible to determine the compositions and mechanical properties of elastically isotropic β-titanium alloys with vanadium and with molybdenum, and to confirm a parabolic dependence of the anisotropy factor on the valence-electrons-per-atom (e/a) ratio. Although a quadratic correlation between the anisotropy factor and e/a was suggested in the second half of the 20th century, the tools available at that time were insufficient to settle the question conclusively.

The thesis also considers plastic strengthening via TWIP/TRIP (Twinning-Induced Plasticity/Transformation-Induced Plasticity) transformations in titanium-based alloys, which have become a particularly attractive research topic in recent years due to their industrial significance. The TWIP/TRIP transformation is highly wanted after in various alloy systems used to manufacture components with a high risk of impact.

In addition to the theoretical studies, the thesis includes experimental results that reveal the key features of an elastically isotropic titanium–vanadium alloy, as well as titanium–niobium—previously unreported. The fabrication and characterization of this class of materials open new route for developing stronger, more fatigue-resistant alloys that enable structural weight reduction.