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Theory-guided design of Ti-based binaries for human implants

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Abstract

State-of-the-art *ab initio* methods constitute a solid basis of modern materials science and materials design. The theoretical research is nowadays increasingly combined with mesoscale and macroscale approaches as well as advanced experimental techniques in order to address complex multiscale and finite-temperature phenomena. The applicability of such a interdisciplinary methodology will be exemplified by our development of novel alloys for human implants, particularly the improvement of hip transplants. The progress in this field is severely hampered by a lack of suitable materials which are biocompatible in terms of non-toxicity and mechanical properties. The aim of our research has been therefore to identify metallurgical trends for non-poisonous Ti-based alloys employing quantum-mechanical calculations. Guided by the theoretical calculations of phase stability and elastic properties, selected alloys were actually melted, cast, and heat treated to a homogeneous state. The samples have been experimentally characterized by x-ray methods and electron microscopy, including crystallographic and chemical analysis, and mechanically tested using ultrasound measurements. The experimental data obtained in these experiments are in excellent agreement with theoretical predictions.

