Author's Accepted Manuscript

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PII: S1751-6161(18)30353-9
DOI: https://doi.org/10.1016/j.jmbbm.2018.08.040
Reference: JMBBM2951

To appear in: *Journal of the Mechanical Behavior of Biomedical Materials*

Received date: 18 March 2018
Revised date: 6 August 2018
Accepted date: 27 August 2018

Cite this article as: P. Kwasniak, J.S. Wróbel and H. Garbacz, Origin of low Young modulus of multicomponent, biomedical Ti alloys - seeking optimal elastic properties through a first principles investigation, *Journal of the Mechanical Behavior of Biomedical Materials,* https://doi.org/10.1016/j.jmbbm.2018.08.040

Origin of low Young modulus of multicomponent, biomedical Ti alloys - seeking optimal elastic properties through a first principles investigation

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Abstract

Multicomponent, biomedical β-Ti alloys offer ultra-low Young modulus values that are related to a unique and poorly understood reduction of C_{44} and C' elastic constants in comparison with binary systems. The elastic properties of such materials are difficult to control due to the large variations occurring even for a small change in chemical composition, which cannot be explained using existing theories. In this article, we investigate the above issues through systematic *ab initio* elastic constants calculations for a series of binary, ternary and quaternary Ti alloys. Special attention is paid to examining the reliability of the methodology adopted and to clarifying the atomic scale mechanisms that affect the mechanical properties of the systems analysed. It was found that the lower boundary of the polycrystalline Young modulus of Ti-Nb-base β phase is close to 50 GPa, and strongly depends on two specific electronic hybridisations related to niobium and simple metals addition that control C_{44} and C'. Based on the relationship established between electronic structure and mechanical properties, we propose several quaternary alloys whose directional <100> Young modulus values are equal or similar to that of human bones. Some electronic-based guidelines for designing new multicomponent β-Ti alloys are also formulated.

Keywords: titanium alloys, ab initio modelling, elastic constants, low Young Modulus

1. Introduction

Recent estimations enclose that about 90% of the population over the age of 40 experiences some kind of degenerative disease related to joints and musculoskeletal disorders [1]. It is expected that, with an increasing elderly population, the number of surgical implants performed will grow steadily. According to the available data, by the year 2030 the number of hip and knee replacements