Abstract Submitted
for the 4CS19 Meeting of
The American Physical Society

The Rational Search for Strong Biocompatible Alloys WADE KLOPPENBURG, Department of Physics, New Mexico State University, JAIME MOYA, EMILIA MOROSAN, Department of Physics and Astronomy, Rice University, KA'AI KAUWE, TAYLOR SPARKS, Department of Materials Science and Engineering, University of Utah, BORIS KIEFER, Department of Physics, New Mexico State University — Materials design, namely the identification of material sets that simultaneously show combinations of desired chemical/physical properties remains challenging. Here we discuss a strategy to find new biomaterials for reconstructive surgery. The relevant design attributes for this application are simultaneous high material strength and ductility. In this respect, it has previously been shown that bulk $\beta Au_{0.25}Ti_{0.75}$ can be stabilized in a phase with a Vicker's hardness that is 3-4 times higher than that for any other Au/Ti ratio. Our Density-Functional-Theory (DFT) computations of the ideal material strength in Au-Ti alloys show the same trend and allow to connect glide system and electronic structure. We expand previous equilibrium computations and discuss the effect of deformation on the electronic structure, a key to rationalize the unusually high strength of this alloy. Combining crystal structure and electronic structure we data mined AFLOW for similar materials. Based on the search results we predict the existence of several novel high strength alloys with possible applications in reconstructive surgery.

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Date submitted: 12 Sep 2019 Electronic form version 1.4