Structural and electronic properties of β Ti-based alloys by density functional theory

D. Fylaktooulou *, Y. Fortouna, A. Balerba, Ch. E. Lekka
Department of Materials Science and Engineering, University of Ioannina
Institute of Materials Science and Computing, Univ.of Ioannina, Ioannina, Greece

The β- Ti-based alloys represent the second generation of biocompatible alloys that are suggested to be promising materials for replacing the widely used TiAl6V4 implants [1-2]. That is since the β- Ti-based netallic implants show lower Young moduli, higher corrosion resistance and minimal cytotoxicity. Nevertheless, in order to retain or improve these features and even include anti-bacteria properties further work is needed. This study consists of a systematic evaluation on the structural and electronic properties of the well known β-TiNb alloys in presence of biocompatible elements like Sn, In, Hf, Ga, Cu, Ag and Zr. Investigations on the ternary TiNbX (X= Sn, In, Ga) revealed that minor In or Sn additions (having sp valence electrons) introduce low energy states with s character that present antibonding features with the Ti first neighboring atoms as well as with the Ti-Nb second neighboring atoms thus weakening the chemical bonds and leading to elastic softening [2,3,4].

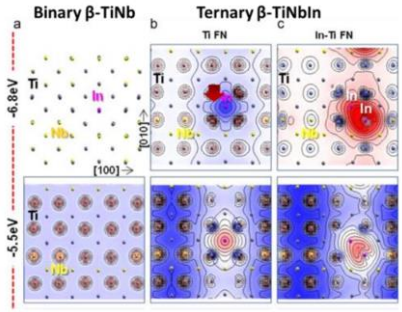

Figure 1: Electronic properties of βTiNbIn based alloys

On the contrary Hf substitution (sd valence electrons) in the orthorhombic Ti-Nb results in a phase transition to the β-phase due to Hf 5d contributions at the Fermi level and the Hf 6s hybridizations at low energies in the electronic density of states. Bonding–anti-bonding first neighbor features existing in the shifted plane destabilize the β-phase, especially at high Hf concentrations, while the covalent-like features in the first neighborhood stabilize the corresponding plane of the _β-phase. New states close to the fermi level are also introduced upon Cu substitution in the β-TiNb alloy. These results could be enlighten the design of β-type Ti-alloys suitable for metallic implants.

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* stm02447@uoi.gr