Biocompatible Titanium-based alloys for orthopaedics

Ch.E. Lekka
Department of Materials Science & Engineering, University of Ioannina, Greece

Medical implants require low Young moduli (E), high corrosion resistance and minimal cytoxicity. BCC Ti-based alloys are promising candidates for replacing the TiAl6V4, which is currently in use. This β-phase can be achieved by the presence of stabilizers (Nb, Mo, Ta, V) resulting in lower E values (in the range 55 to 85GPa). Nevertheless, these values are still far from the desirable one for bone replacing material that should not exceed 30GPa. The E reduction, e.g. the β-Ti-xNb, (x<40w% above which the E increases) could be further improved by suitable additional non-toxic elements (e.g. In, Sn, Hf). Unfortunately, although at high temperatures, the β-TiNb is favoured, upon quenching and below 40w% several phases may coexist (α, β, α'' and ω), thus impeding E lowering. Aiming in a fundamental understanding of the relationship between structural and mechanical properties of Ti-Nb phases, we performed a detailed theoretical analysis seeking for the electronic origin of structural instabilities. We found that upon Nb enrichment the unit cell increases, a result that is associated with an enhancement of the number of d-electrons, especially around -1eV, and the depletion of the occupied electronic states at the Fermi level, which characterize the β-phase of Ti, thus leading in stable β structure. Moreover, we revealed correlations between the β-phase electronic band structure characteristics at specific k-points that are related to the well known Ti soft phonon modes.
The presence of low content <6.25at%) In or Sn p-electron dopant in the Ti-25at %Nb introduces low energy states (around -8eV) with anti-bonding characteristics with the first and second neighbouring atoms, thus weakening the chemical bonds, in line with experimental findings that suggest lowering of the Young modulus. At high Sn (or In) concentration (>12.5at%), first or second neighbourhood may include Sn-Sn pairs that exhibit strong direction bonds at even lower energy states, thus increasing the Young modulus.
These results could be of use for the design of low stiffness biocompatible alloys.

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