Ab initio calculations on β Ti-based implant surfaces

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Implant surfaces are really critical for tissue engineering, osteogenesis as well as bacterial adhesion and proliferation [1-2]. Usually, polymeric coatings have been widely used for the manufacturing of the medical device's surfaces in order to tune the mechanical properties and biocompatibility. Nevertheless, the knowledge of the properties of the metallic implant or the oxide termination that will affect any coating adsorption or even bacteria deposition is critical. Therefore, aiming in a fundamental understanding of metallic implant surfaces, a detail study on the structural and electronic properties β- Ti based alloy surfaces with non-toxic and antibacterial element enrichment is needed. In this work a detail study of several β-TiX (X=Nb, Ga, Cu, Ag) low index surfaces in presence of antibacterial adatoms is presented. The energetically favored terminated layer is revealed for the order or disorder (001) and (110) surfaces. Surface contraction is found for all cases and the rippling effect is revealed for the mix terminated layers. Surface atoms introduce new surface energy states altering the bulk electronic density of states while the adatoms mainly interact with the Ti surface atoms.

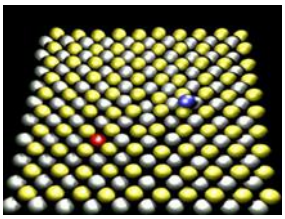

Figure 1: Metallic β-TiNb (110) surface in presence of Ga adatom

Furthermore, the structural and electronic properties of TiO_2 anatase and rutile surfaces are presented since this oxide layer is usually formed ontop of any Ti-based implant.
These results can be used as a guide for the design of novel low-rigidity alloys for biomedical applications.

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References

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