General comments: Major revision.

Abstratct and title speaks to the content, but technical corrections must be made to abstract.

Technical corrections of the abstract have been revised as follows:

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1. Statements and in general paper is poorly referenced

- The use of Titanium (Ti) and Ti-based alloys implantable device has become a great part of modern medicine [1]. Compared to other metallic implants (stainless steel and cobalt-chromium) Ti-based alloys stands out with its unique properties which makes it more probable for prosthetic applications [2]

2. The authors makes certain statements without properly discussion or referencing. These are indicated in the scanned copy. This is seen throughout manuscript.

The statements have been revised and discussed as follows:

- The Brillouin zone integrations were performed for suitably large sets of *k*-points according to Monkhorst and Pack [14]. The solid solution approach employing visual crystal approximation (VCA) [15] embedded in CASTEP was used to substitute Ti with Mo atoms. It is a much simpler and computationally less expensive approach in which one studies a crystal with the primitive periodicity but composed of fictitious ‘‘virtual’’ atoms that interpolate between the behavior of the atoms in the parent compounds. This technique has seen wide use in band structure calculations [16, 17, 18]

3. Add a figure of lattice parameters as function of Mo concentration and then elaborate on the figure in the text.

A Figure of young modulus as a function of Mo concentration of the study and experimental results was added instead of the lattice parameters. This is because the study objective is to stabilise the β Titanium to find Young’s modulus close to the bone. The Figure has been added and discussed as follows:

- Figure 2 represent the Young’s moduli of the calculated and experimental Ti-Mo with respect to the varying Mo concentration. In fig 2 the experimental Young’s modulus decreased with the addition of Mo, although the actual value of the modulus fluctuated with different Mo concentration which was due to the presence of metastable phases α″ and ω in some of the samples during the XRD and TEM investigation [19]. Interestingly the theoretical and experimental Young modulus show a similar trend, they both increase with increasing Mo content showing structural stability. It is also observed that the Youngs modulus of Ti92Mo8 in the reported study was low (61GPa) which was in good agreement with Sung experimental observations [19]. It is noted that the Young’s modulus of the experimental result was larger than that of the theoretical calculations this is because the theoretical calculations were restricted to bulk single crystals, while the real samples are polycrystalline [20-21]. The difference might also be due to the difference in temperature (0K for all calculations and 298K for experimental).

4. Under the DOS section should provide more detailed discussion and comparison to other work. How does the theoretical work in this paper compare to some other experimental work? There must be experimental work that can be used for comparison

The Dos has been revised as follows:

- The embedded total density of states is represented in figure 4. We note that the TDOS peak of pure titanium although with lower density of states near Ef it is much broader than the other peaks and located in the antibonding region. Interestingly at 8 at. % Mo concentration, the dip of the TDOS at Ef was observed to slightly move away from the antibonding region suggesting β-phase stability increased gradually. Lower number of density of states was observed for $Ti_{92}Mo_8$ plot at Ef compared to the other structures confirming it to be the most stable structure. However, it was noted that $Ti_{90}Mo_{10}$ is the least stable structure since it has the highest number of density of states at Ef. Our DOS analysis is in good agreement with some theoretical studies which suggest that the DOS at Ef decreased with increasing Mo content for ordered cells, indicating that the β-phase stability. The opposite is observed for distorted cells where by Li et al observed that higher Mo content produces the most stable structure [23].

5. Fig 2 forms the core of the work; however, it is not properly discussed in the text.

Figure 2 has been revised and discussed as follows:

- Structural instability is related to the Fermi level (Ef) which is represented by the vertical line in fig 3 below. According to Mahlangu et al [22] structures with the highest and lowest density of states at E_f is considered the least and most stable, respectively. It is very clear from fig 3 that the s and p orbitals peaks are much broader than sharp peaks observed for the d orbital at Ef. We also observe in fig 3b, c and d that d-orbital of Mo has the major contribution to the TDOS near Fermi level.