Computational modelling of $Ti_{50}Pd_{50-x}Cu_x$ (0≤x≤25) high temperature shape memory alloys

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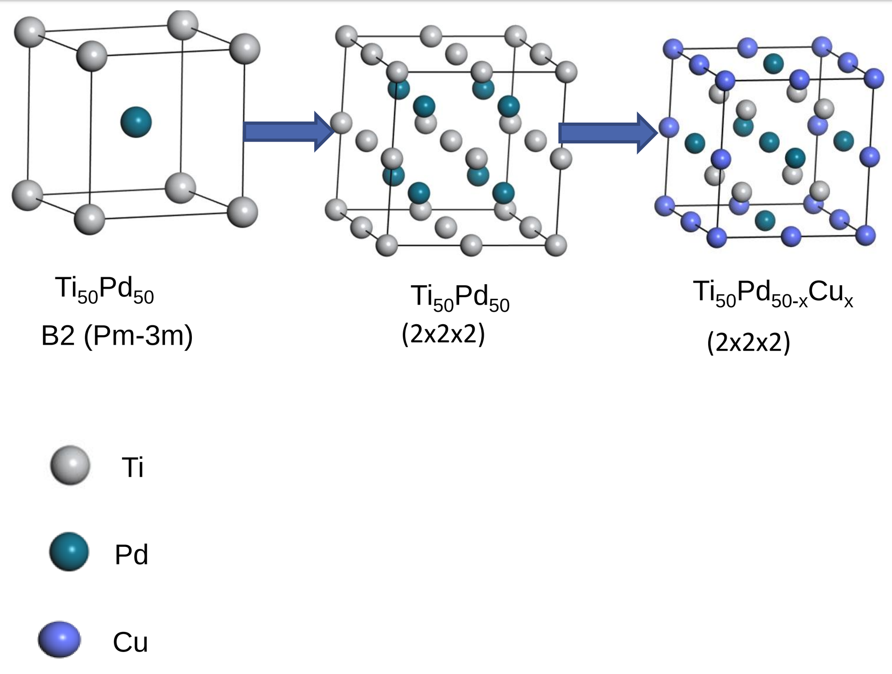
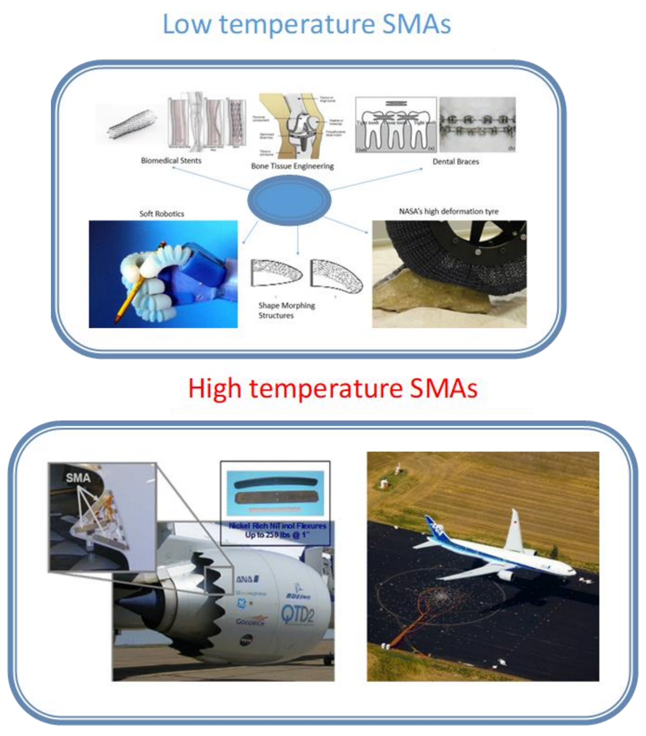
Introduction

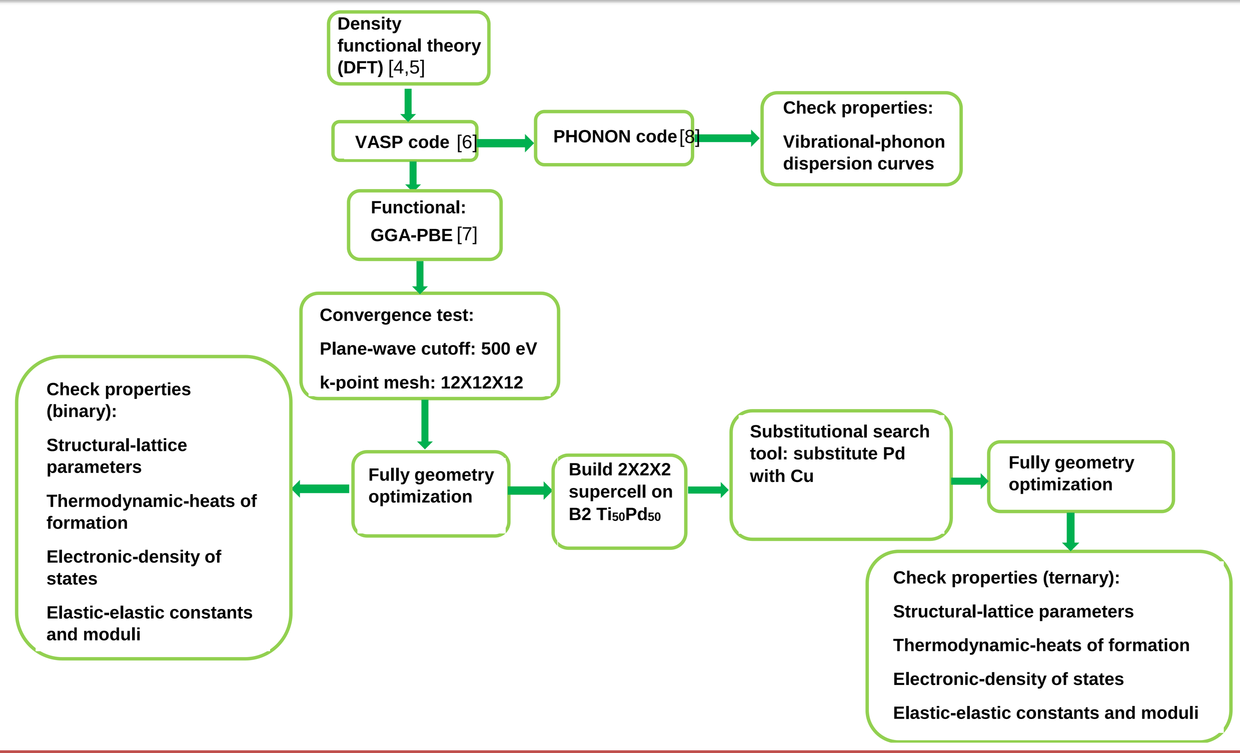
Titanium-based alloys in particular $Ti_{50}Pd_{50}$ are being developed for high temperature applications. The $Ti_{50}Pd_{50}$ alloy has a potential for high temperature shape memory applications due to its martensitic transformation capability from B2 to B19 at 823 K [1]. This alloy exists as a high temperature phase (austenite phase) which has a simple cubic B2 while at low temperature is known as the martensite phase with an orthorhombic B19 structure [2]. Previous studies indicated that B2 TiPd is unstable displaying a negative C' at 0 K [3]. Consequently, the binary $Ti_{50}Pd_{50}$ alloy has no strength for use in actuators and aeronautic industry and ternary alloys need to be established to improve their properties Then, alloying with Cu is an attempt to improve their strength at 0 K as it has extraordinary properties such as corrosion resistance and high thermal conductivity. In this study, ternary alloying of $Ti_{50}Pd_{50}$ with Cu have been performed using DFT approach to investigate the thermodynamic an d mechanical stability to deduce their potential in HT application.

Structures and Applications





Methodology



Results and Discussions

Structural and thermodynamic properties

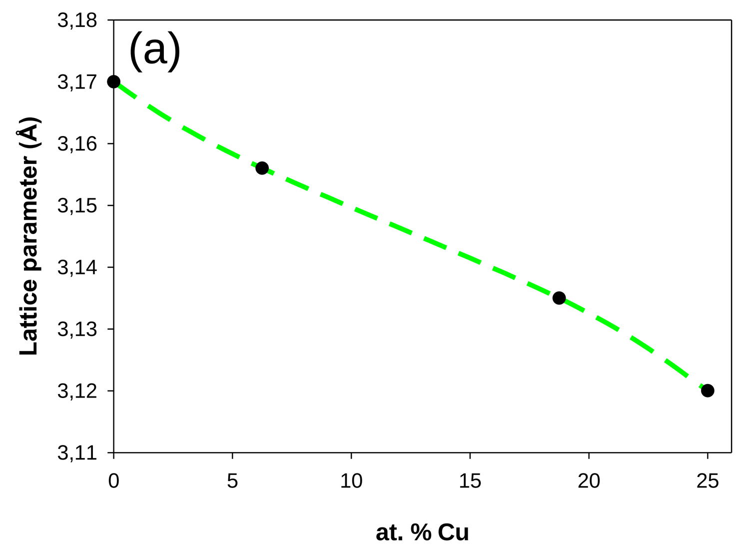
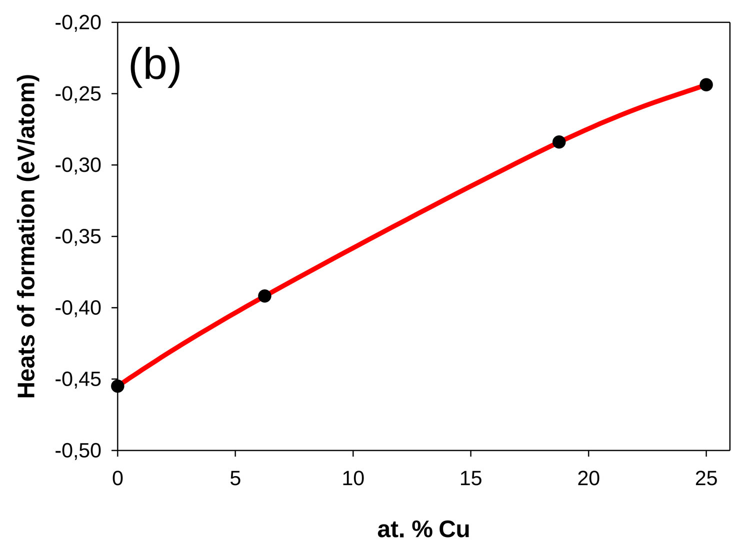


Figure 1 (a): It is clear that the lattice parameter decreases as Cu content is increased, this is attributed to the small radius of Cu compared to Pd.



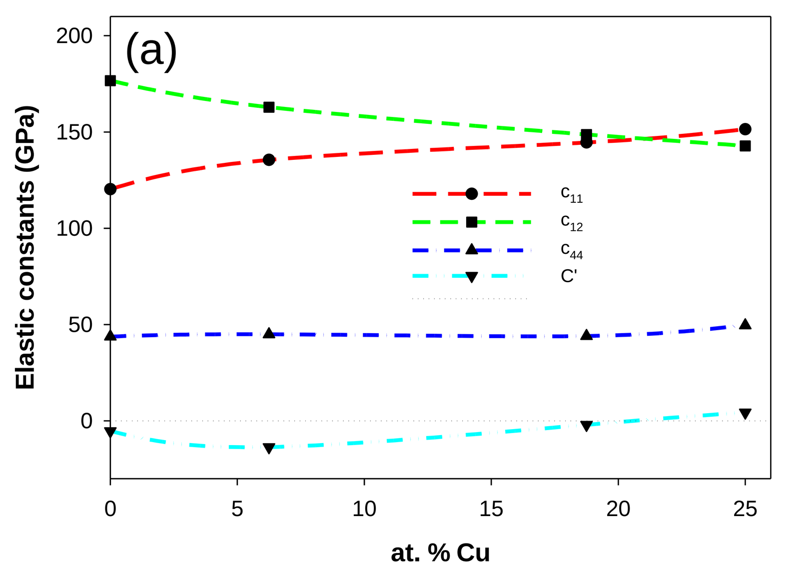
The heat of formation is determined by expression:

$$\Delta H_f = E_C - \sum_i x_i E_i$$

For a structure to be stable, the heat of formation must have the lowest negative value ($\Delta H_f < 0$). **Figure 1 (b):** It is clearly seen that the heat of formation decreases as the concentration of Cu is increased. At 6.25 at. % Cu, the ΔHf is the lowest which implies thermodynamically stable compared to other Cu compositions such as 18.75 and 25..

Figure 1: (a) Lattice parameter, a (Å) and (b) heats of formation of the B2 $Ti_{50}Pd_{50-x}Cu_x$ (0≤x≤25) ternary SMAs.

Elastic properties



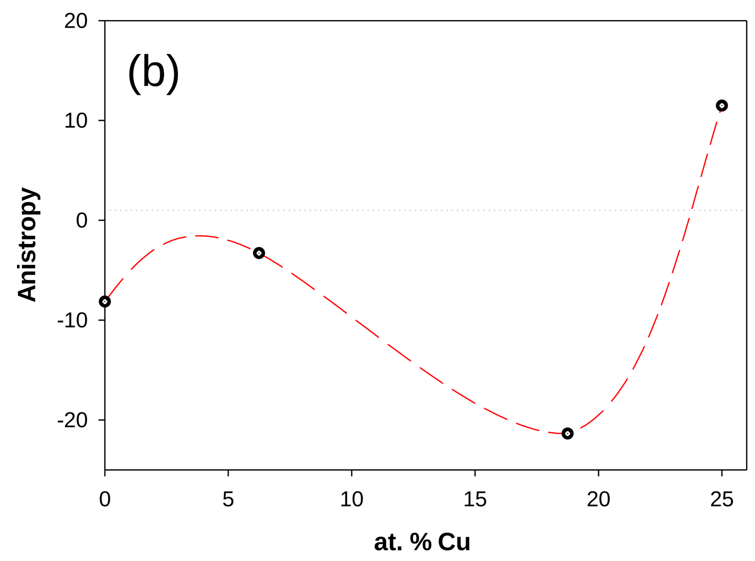
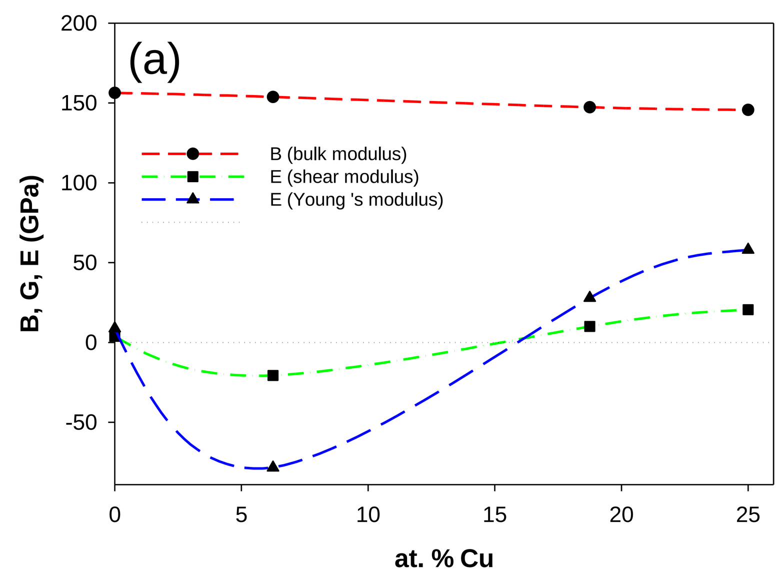


Figure 2: (a) elastic constants (GPa) and (b) anisotropy as a function of atomic percent Cu for $Ti_{50}Pd_{50-x}Cu_x$ where 0 ≤ x ≤ 25.

The mechanical stability condition for cubic system [9]: $C_{11} > C_{12}, C_{44} > 0$, $C' = \frac{1}{2}(C_{11} - C_{12})$, $C' > 0$
For an isotropic crystal, the factor (A) must be 1, while any value small or large than unity is a measure of the degree of elastic anisotropy. Anisotropy ratio is determined from $A = \frac{C_{44}}{C'}$
Figure 2 (a): It is observed that B2 $Ti_{50}Pd_{50-x}Cu_x$ is mechanical stable above 25 at. % Cu.
Figure 2 (b): It is clearly seen that $Ti_{50}Pd_{50-x}Cu_x$ show anisotropic behaviour for 0 ≤ x ≤ 25.

Hardness and ductility



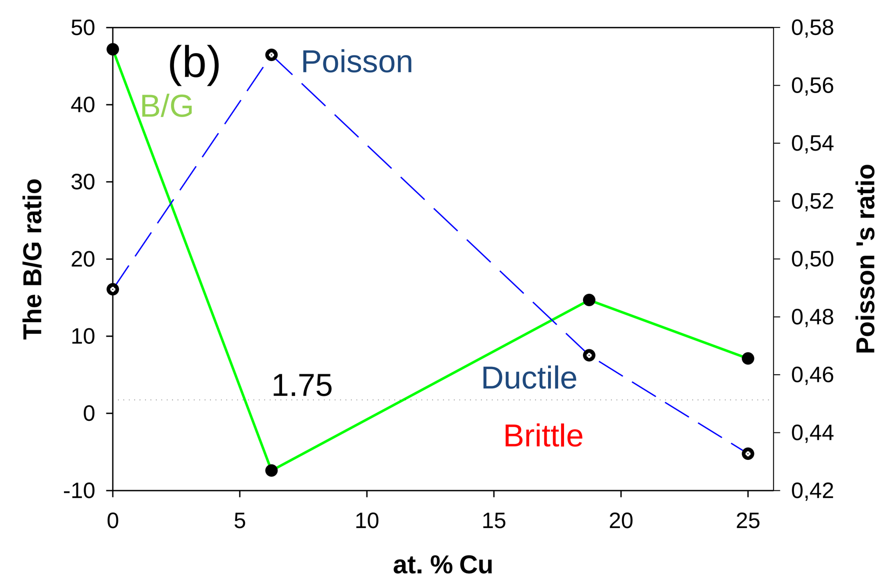


Figure 3: Simulated (a) Bulk (B), Shear (G), Young 's modulus and (b) The B/G ratio, Poisson 's ratio as a function of atomic percent Cu for $Ti_{50}Pd_{50-x}Cu_x$ (0 ≤ x ≤ 25) SMAs.

Figure 3 (a): The bulk modulus decreases minimally with an increase in Cu concentration. $Ti_{50}Pd_{43.75}Cu_{6.25}$ appears to be the hardest due to the highest bulk modulus as compared to other compositions. The G and E is greater than above 18 at. % Cu which indicate that the structure is less compressible and stiffer.
Ductility condition:
The Pugh (B/G) > 1.75 [10] and Poisson (σ)> 0.26 [11] is regarded as ductile otherwise brittle.
In **Figure 3 (b)**, the B/G ratio >1.75 except for 6.25 at. % Cu (condition of ductility). In the case of Poisson 's ratio, the ductility is observed for (0 ≤ x ≤ 25) as the ratio is greater than 0.26.

Phonon dispersion curves

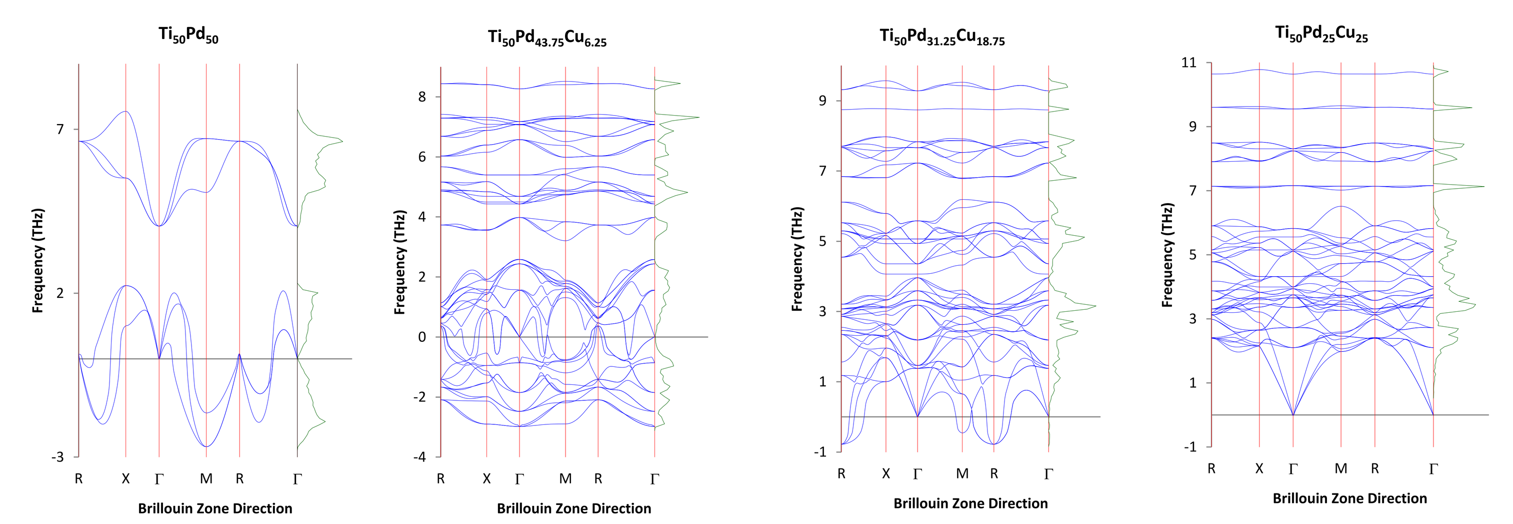


Figure 4: The phonon dispersion curves of the $Ti_{50}Pd_{50-x}Cu_x$ (0 ≤ x ≤ 25) ternary structures.

Figure 4: The phonon dispersion curves of $Ti_{50}Pd_{50-x}Cu_x$ show no negative vibrational frequencies above 20 at. % Cu suggesting that the material is vibrational stable. The other phonon dispersion curves are vibrational unstable displaying soft modes along gamma point which correspond with their negative Shear moduli (C') for (0 ≤ x ≤ 18.75) .

Conclusion

Ab initio DFT approach was successfully used to study SMA properties of B2 $Ti_{50}Pd_{50-x}Cu_x$ for potential HT applications. The results suggest that $Ti_{50}Pd_{50-x}Cu_x$ are thermodynamically stable fat lower composition (6.25 at.% cu) with the lowest value of the heats of formation. The effect of ternary addition revealed that $Ti_{50}Pd_{50-x}Cu_x$ alloys are mechanically stable above 20 at. % Cu according to the criteria of mechanical stability. Cu addition was found to increase the martensitic transformation temperature of the TiPd since it gives the negative C' below 20 at. %. It was revealed that increasing Cu above 6.25 at. % could effectively improve the ductility of the compound. Our phonon dispersion calculations predicted vibrationally instability below 18.75 at. % Cu

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Acknowledgments

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