Effect of Ti content on the magnetic and mechanical properties of B2 FeCo alloy: a DFT study

T M Ledwaba, R G Diale, P E Ngoepe and H R Chauke

University of Limpopo, Materials Modelling Centre, Private Bag x1106, Sovenga, 0727

E-mail: tebogo.ledwaba@ul.ac.za

Abstract. Iron-cobalt alloys are considered a good candidate for high-temperature applications due to their high saturation magnetization and Curie temperature. These alloys are applicable in the automotive industry as actuators, however, suffer low levels of ductility at room temperature. In this study, ternary alloying is used to investigate the strength of the alloys. Titanium is chosen as the alloying element since it has the potential to enhance the ductility of the alloy system. A density functional theory study applying the supercell approach was used to investigate the stability and magnetic behaviour of B2 $Fe_{50}Co_{50-X}Ti_X$ ($0 \leq X \leq 50$) structures. Full structural optimization have been performed and provided equilibrium ground-state properties for both binary and ternary system in good agreement with previous studies to with 1 %. The stability of $Fe_{50}Co_{50-X}Ti_X$ is evaluated from the formation energies, elastic properties, magnetic properties and phonon dispersion curves. We find that the thermodynamic stability increases with an increase in Ti content. Furthermore, the calculated Pugh's and Poisson's ratios showed that alloying with Ti effectively enhances ductility. Moreover, $Fe_{50}Co_{50-X}Ti_X$ systems showed positive shear modulus for the entire concentration range, a condition of mechanical stability. It was also revealed that the Ti addition does not compromise the magnetic properties of the alloy greatly. Thus, the results suggest that the B2 $Fe_{50}Co_{50-X}Ti_X$ alloy can be used for the development of magnetic components with good strength that can be used for actuator applications.

1. Introduction

Fe-Co alloys represent a crucial group of soft magnetic materials [1, 2, 3] which provides remarkable magnetic properties due to their scarce combination of good properties such as high mechanical strength, low coercivity, high permeability, and highest saturation magnetization. [4]. These alloys find application in pole tips for high field magnets, data storage, and high-performance transformers [5]. They also have the potential for use in the manufacturing of aircraft and jet engines, but they are rarely used due to their low levels of ductility at room temperature [6]. The workability of these alloys can be improved by ternary additions which may lead to higher tensile strength and elongation at room temperature.

Ternary alloying with Pd was investigated previously to improve the ductility of FeCo [7]. However, no information was given on how this affected the magnetic properties of the material since Pd reduced a considerable amount of Fe, which may lead to weak magnetic properties. In another study, it was reported that the addition of vanadium on the B2 Fe-Co alloy relieved the poor ductility and facilitated hot rolling in the disordered state by up to 90 %. Comparable to other alloying elements, adding vanadium to Fe-Co alloy weakens its magnetic properties [4]. In this study, we have used the plane-wave implementation of density functional theory (DFT) to investigate how ternary alloying can

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improve the ductility of a typical bimetallic alloy, i.e. FeCo. Titanium was chosen as the alloying element since it has the potential to enhance the ductility of the alloy system without compromising the magnetic strength [8]. Furthermore, structural, mechanical, and thermodynamic properties were evaluated to ascertain the influence of Ti addition in the FeCo system.

2. Methodology

The calculations were carried out using the Vienna ab initio simulation package (VASP) code [9] based on density functional theory [10, 11] along with the projector augmented wave (PAW) pseudopotential [12]. We have used the generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional [13] since it provided better results compared to other functionals. An energy cut-off of 500 eV was used, to achieve a good convergence of the parameters. The k-spacing of 0.2 1/Å (12X12X12) for B2 FeCo was used according to Monkhorst and Pack [14]. A 2x2x2 B2 $Fe_{50}Co_{50}$ supercell was used to generate different compositions (6.25, 18.75, 25, 31.25 and 43.75 at. % Ti). The most favorable Co substation-sites were chosen based on the lowest possible total energy values i.e. the structure with the lowest energy was considered for each concentration. Note that the Pm-3m symmetry was maintained in all calculations since there was no significant difference with the results of the P1 symmetry. The structures were fully relaxed with respect to the volume, shape and internal atomic positions until the atomic forces were less than 0.01 eV/Å.. Their stability was evaluated using heats of formation and the Born elastic stability criteria [17,18]. All calculations were subjected to spin polarization to take account of the magnetization. The PHONON [26] code was used to determine the phonon dispersion curves of both binary and ternary systems. The atomic arrangements of pure FeCo and supercell are shown in figure 1.

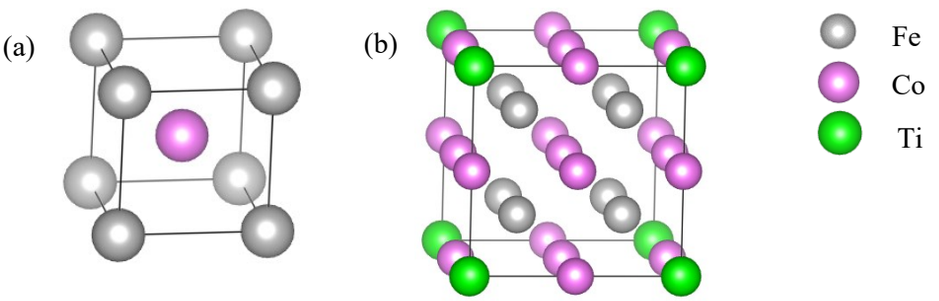

Figure 1. The atomic arrangements of the unit cell (a) binary B2 FeCo (b) B2 FeCo-Ti (2x2x2 supercell) with the space group Pm-3m.

3. Results and discussions

3.1. Structural and thermodynamic properties

Figure 2 shows the equilibrium lattice parameters for the $Fe_{50}Co_{50-x}Ti_x$ ($0 \leq x \leq 50$) alloys. The equilibrium lattice parameter of binary B2 FeCo was predicted to be 2.844 Å (2.840 Å [16]) which agrees very well with experimental data to within 1 %. It was noted that the lattice parameter of the $Fe_{50}Co_{50-x}Ti_x$ decreases as Ti content is increased (see figure 2).). This is due to the large atomic radius of Ti (1.76 Å [27]) compared to Co (1.52 Å [28]). The thermodynamic stability of $Fe_{50}Co_{50-x}Ti_x$ is argued through the predicted heats of formation (ΔHf). ΔHf was calculated by subtracting the individual atomic energies (Fe, Co, Ti) from that of the bulk system:

$$\Delta H_f = E_C - \sum_i x_i E_i, \quad (1)$$

where E_C is the calculated total energy of the compound and E_i is the calculated total energy of the element in the compound. Note that for a structure to be stable, the heat of formation must have the lowest negative value ($\Delta H_f < 0$) otherwise, a positive value implies instability. In figure 3, we show the heats of formation for the B2 $Fe_{50}Co_{50-x}Ti_x$ systems for concentrations $0 \leq x \leq 50$. The heats of formations for the binary B2 $Fe_{50}Co_{50}$ was found to be -0.057 eV/atom (-0.065eV/atom [25]) which is in good

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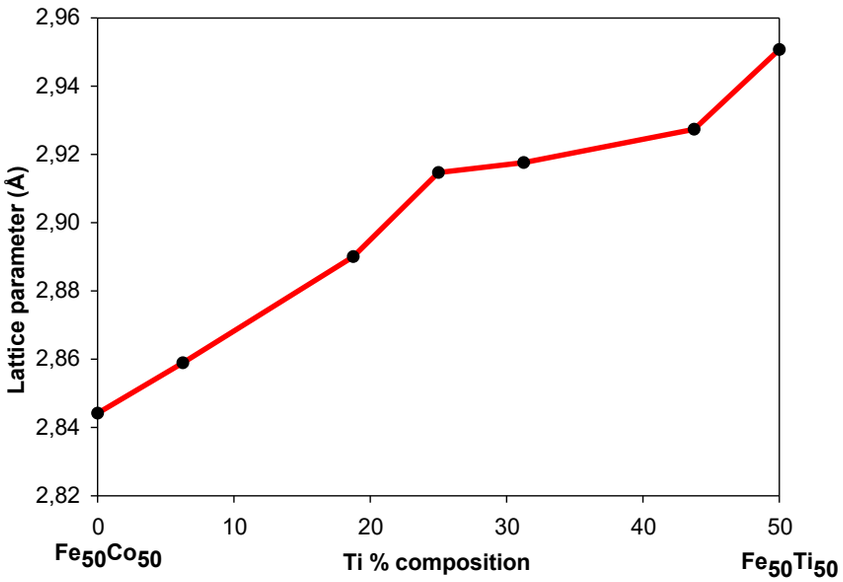

Figure 2. Lattice parameter (Å) against atomic percent Ti for $Fe_{50}Co_{50-X}Ti_X$ alloys ($0 \leq x \leq 50$).

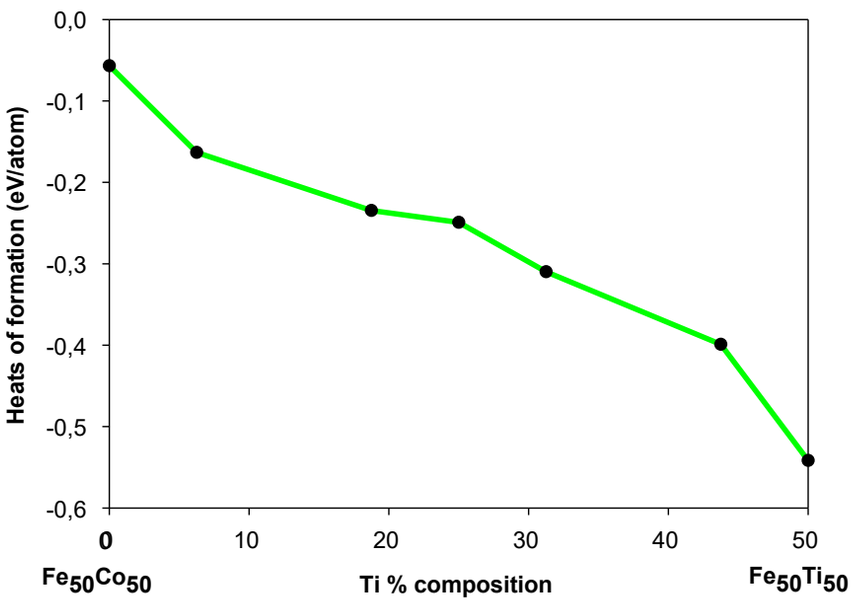

Figure 3. Heats of formation, ΔHf against atomic percent Ti for $Fe_{50}Co_{50-X}Ti_X$ alloys ($0 \leq x \leq 50$).

3.2. *Elastic and magnetic properties*

The elastic properties give important information about the mechanical stability of compounds. For a cubic crystal structure (i.e B2 $Fe_{50}Co_{50-x}Ti_x$), there are three independent elastic constants (C_{11}, C_{12} and C_{44}), in which case the structure is considered stable if it satisfies the cubic stability criterion as described elsewhere [17, 18]:

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$$C_{11} > c_{12}, C_{44} > 0, \text{ and } C_{11} + 2C_{12} > 0, \quad (2)$$

$$C' = \frac{1}{2}(C_{11} - C_{12}) > 0$$

In figure 4, it is seen that all the independent elastic constants are positive, confirming that the $Fe_{50}Co_{50-x}Ti_x$ alloys are stable in the entire composition range. More importantly, the C' is positive ($C'>0$) which indicates mechanical stability. The C' is slowly varying (at low concentration) and increases slightly with the increase in Ti concentration above 25 at.%. This trend is similar to that of C_{11}, however, the C_{11} plot is higher. We also observe a coupling of C' and C_{44} at about 35 at. % Ti, while C' coincide with C_{12} at about 43.75 at. % Ti. This is attributed to a possible phase transformation from B2 to B19, similar observations were reported previously [24].

To measure the ductility of the materials, we have calculated the Pugh (B/G) and Poisson's ratios as shown in Figure 5 (a) and (b), respectively. Note that a structure is considered ductile if the B/G ratio is greater than 1.75 and otherwise brittle as noted elsewhere [19]. The structures (see figure 5(a)) were observed to be ductile for the entire concentration range since all ratios were greater than the critical value of 1.75.

Poisson's ratio (σ) was also evaluated to confirm the ductility of the material. Note that the structure is considered ductile when σ is greater than 0.26 otherwise brittle [20]. As the content of Ti is increased, the σ values were found to be greater than 0.26 in the entire concentration that is a condition of ductility (see figure 5 (b)).

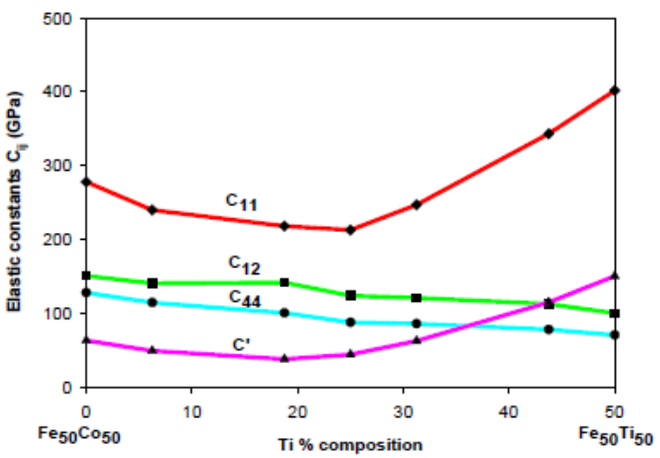

Figure 4. Elastic constants (GPa) against atomic percent Ti for $Fe_{50}Co_{50-X}Ti_X$ alloys ($0 \leq x \leq 50$).

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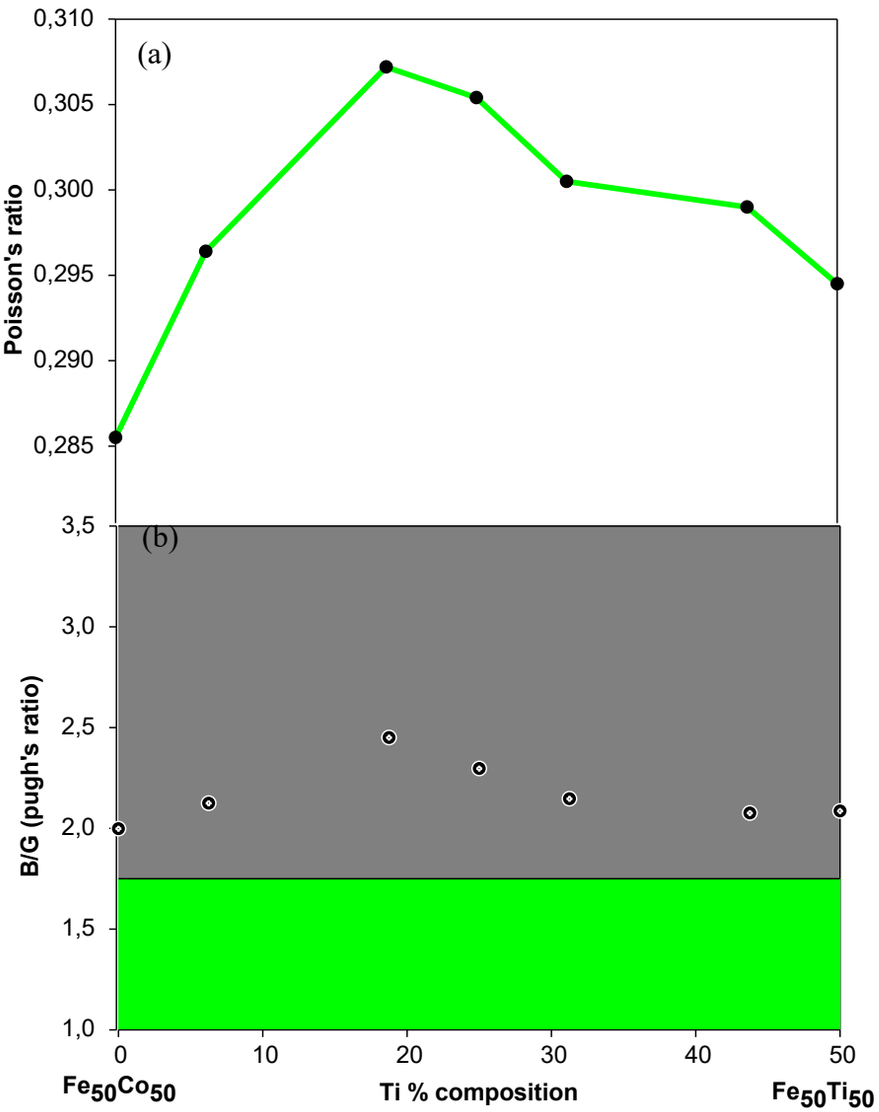

Figure 5. (a) B/G ratio and (b) Poisson's ratio against atomic percent Ti for $Fe_{50}Co_{50-X}Ti_X$ alloys ($0 \leq x \leq 50$).

The total magnetic moments were calculated to check the magnetic strength of both binary $Fe_{50}Co_{50}$ and ternary $Fe_{50}Co_{50-x}Ti_x$ systems. A positive value of total magnetic moment indicates good magnetic strength. The initial magnetic moments were defined for every atom by assigning a chosen value for Fe (3 μB) and Co (2 μB). Figure 6 shows the total magnetic moments of $Fe_{50}Co_{50-x}Ti_x$ alloys as a function of Ti atomic composition. The contributions for each element in the system are also shown and indicate poor magnetic strength for Ti (low magnetic moments), and highest for Fe. The total magnetic moment of the binary B2 $Fe_{50}Co_{50}$ alloy was found to be 4.530 μB in good agreement with the theoretical value of 4.479 μB [25]. It can be seen that the total magnetic moment decrease with an increase in Ti composition. At 43.75 at. % Ti (0 μB), the structure transition from ferromagnetic to diamagnetic, similar observations were discussed elsewhere [29, 30].

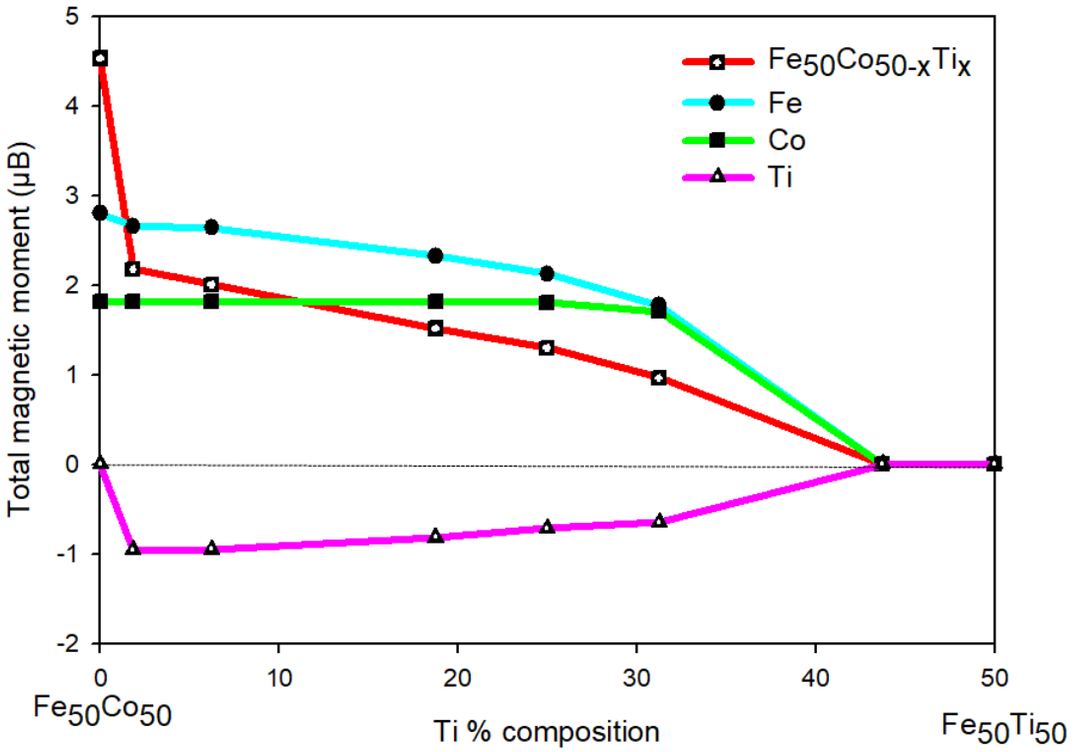

Figure 6. Total magnetic moments against atomic percent Ti for $Fe_{50}Co_{50-X}Ti_X$ alloys ($0 \leq x \leq 50$). The contributions of the individual elements (Fe, Co, Ti) are also included for reference.

3.3. Phonon dispersion curves

The Phonon dispersion curves were calculated to determine the structural stability of B2 $Fe_{50}Co_{50-x}Ti_x$ alloys and are illustrated in figure 7. It can be seen that the phonon dispersion curves of B2 $Fe_{50}Co_{50-x}Ti_x$ are vibrational stable for the entire concentration range ($0 \leq x \leq 50$) due to the absence of soft modes (i.e., negative frequency) along all the Brillouin zone directions. This observation suggests that Ti addition does not compromise the stability of the B2 $Fe_{50}Co_{50}$ structure, and this prediction is consistent with the elastic moduli Cij that are given in figure 4.

3. Conclusion

The DFT results revealed a significant effect of Ti content on the structural, magnetic, and mechanical properties of B2 FeCo alloy. The results showed that $Fe_{50}Co_{50-x}Ti_x$ is thermodynamically stable at high concentrations displaying the lowest heats of formation value. It was found that $Fe_{50}Co_{50-x}Ti_x$ alloys are mechanically stable for the entire concentrations according to the cubic stability criteria. Furthermore, the ductility is enhanced due to an increased tendency in the Pugh (B/G) and Poisson ′s ratio with an increase in Ti concentration above the critical point. The phonon dispersion curves showed mechanical stability for the entire concentration of $Fe_{50}Co_{50-x}Ti_x$ ($0 \leq x \leq 50$). Ternary addition of Ti slightly reduces the total magnetic moments of B2 FeCo, however, maintained the magnetic strength as well as the mechanical stability. The present findings may guide the future development of Ferromagnets made up of new $Fe_{50}Co_{50-x}Ti_x$ alloys.

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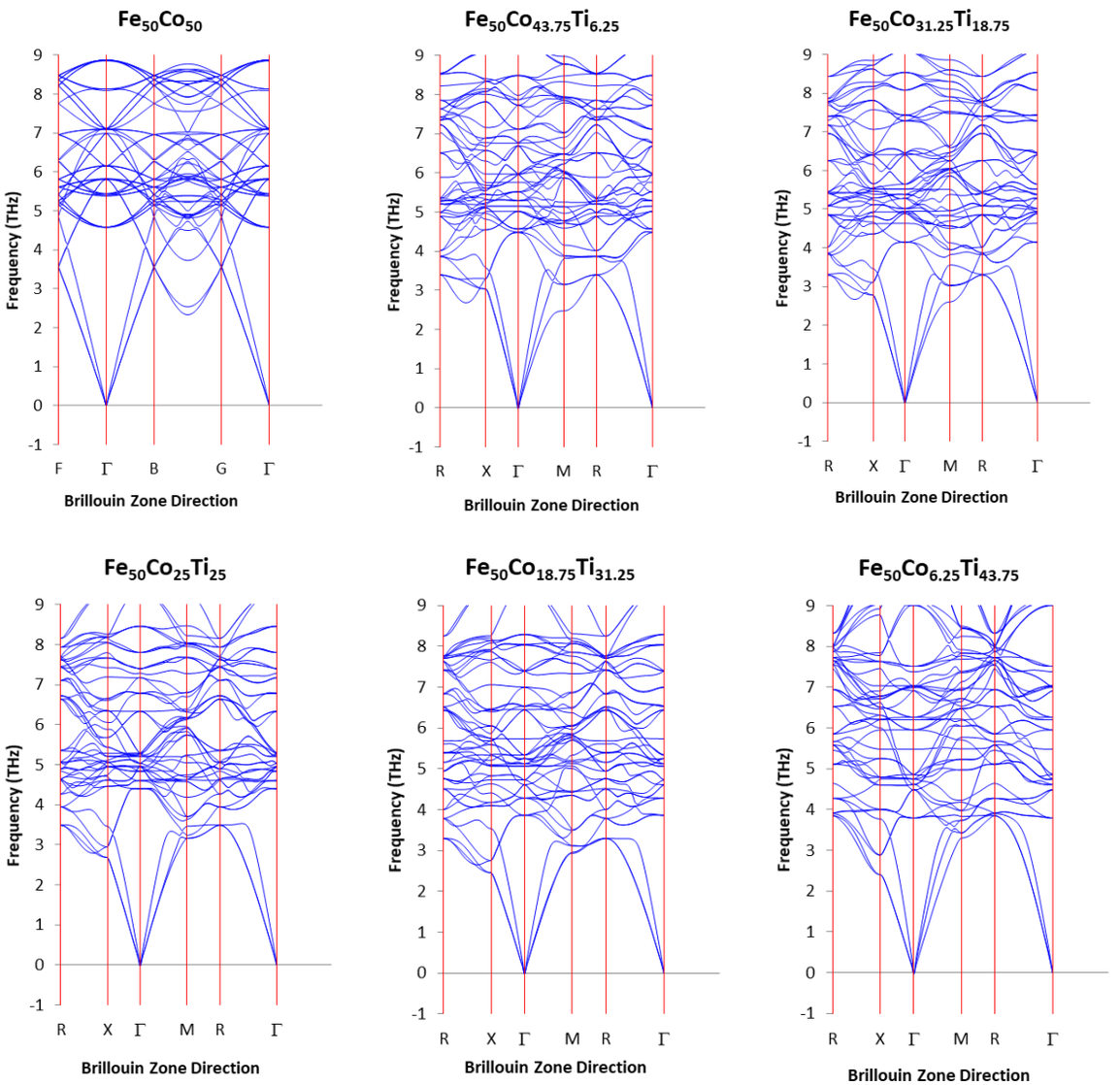

Figure 7. Phonon dispersion curves for B2 $Fe_{50}Co_{50-x}Ti_x$ alloys, where $0 \leq x \leq 43.75$ and the Γ (000) denote the center of the Brillouin zone.

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