Ti content on the magnetic and mechanical properties of B2 FeCo alloy: A computational study.

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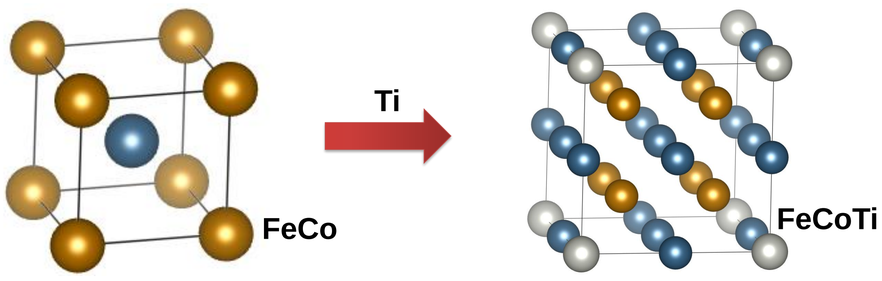
SAIP 2021 South African Institute of Physics Conference

Introduction

FeCo alloy offers exceptional magnetic properties because of their rare combination of improved properties such as high mechanical strength and soft magnetic character, with high permeability, high Curie temperature, high tensile strength and the highest saturation magnetization of all known magnetic alloys which are required for advanced power applications [1]. FeCo magnetic particles are considered attractive materials in various engineering applications owing to their superior properties, particularly their high saturation magnetization. However, the B2 binary FeCo suffers poor ductility at room temperature, which makes this alloy difficult to process [2]. Due to their smooth magnetic characteristics at elevated temperatures, there is a lengthy tradition of using FeCo alloys with ternary element additions as engineering materials [3]. The workability of these alloys can be improved by adding titanium which leads to a higher tensile strength and elongation at room temperature. By combining the soft magnetic properties of iron and hard magnetic properties of cobalt and titanium, an optimal magnetic material could be developed. Titanium has low density, high strength, and it is resistant to corrosion. In this study, ternary alloying of FeCo with Ti has been performed using DFT approach to investigate the thermodynamic, mechanical and magnetic stability.

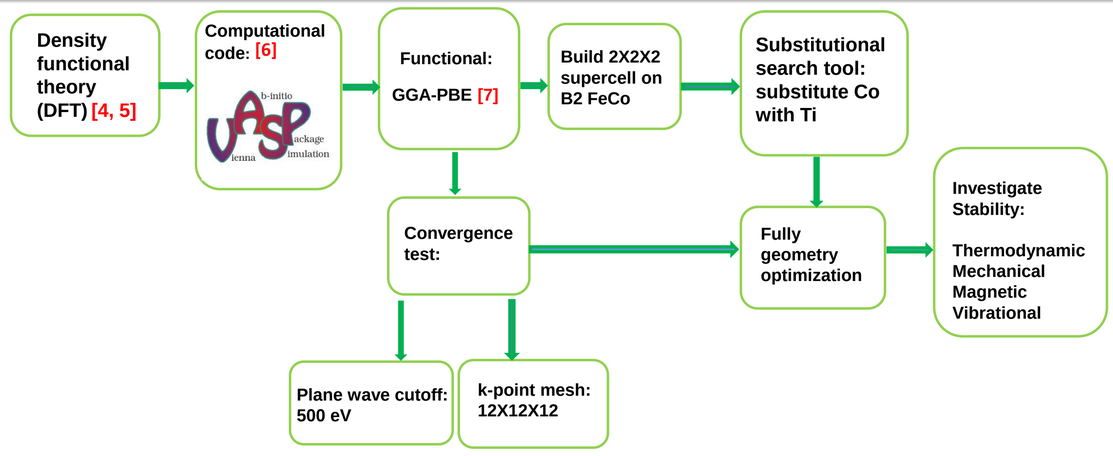
Structures and Applications



Jet engine

Generator for aircrafts

Methodology



Results and Discussions

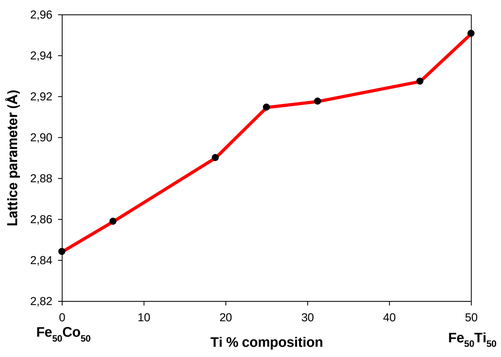


Figure.1 Lattice parameters for $Fe_{50}Co_{50-x}Ti_x$ against atomic % composition

In **Figure 1,** the lattice parameter increases as Ti content is increased, this is due to the large atomic radius of Ti compared to Co.

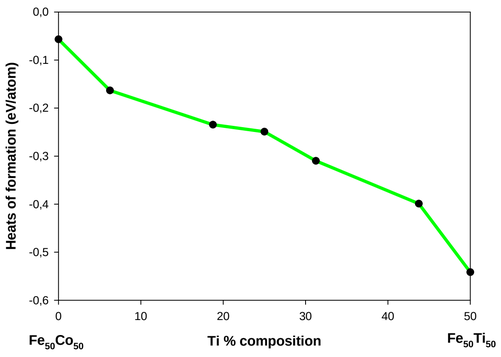


Figure. 2 Heats of formation for $Fe_{50}Co_{50-x}Ti_x$ against atomic % composition

The least value for heat of formation (ΔH_f) is the most stable. In **Figure 2,** we observe that as Ti content is increased, ΔHf decreases. This implies that the structure becomes thermodynamically stable with the addition of Ti.

Elastic Properties

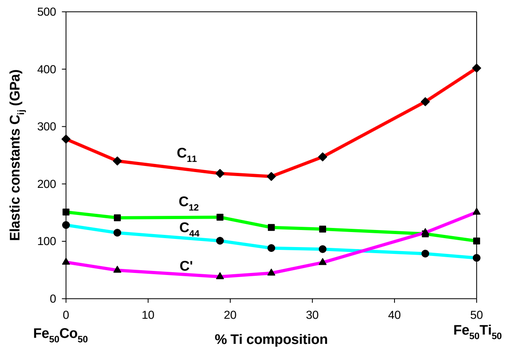


Figure. 3 Elastic constants (GPa) as a function of atomic percent (at. %) Ti for $Fe_{50}Co_{50-x}Ti_x$

The mechanical stability condition for cubic system: $C_{11} > C_{12}, C_{44} > 0, \; C' > 0$.

Figure. 3 show that the mechanical stability conditions are satisfied for the entire concentrations of $Fe_{50}Co_{50-x}Ti_x$ alloys where ($0 \leq x \leq 50$).

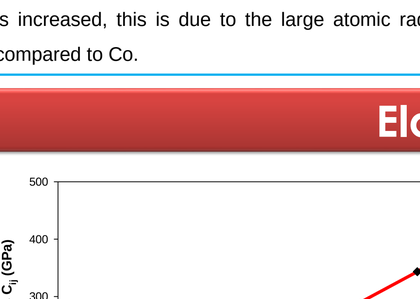


Figure. 5 Magnetic moments (*Bohr magneton*) as a function of atomic percent Ti for $Fe_{50}Co_{50-x}Ti_x$ alloys.

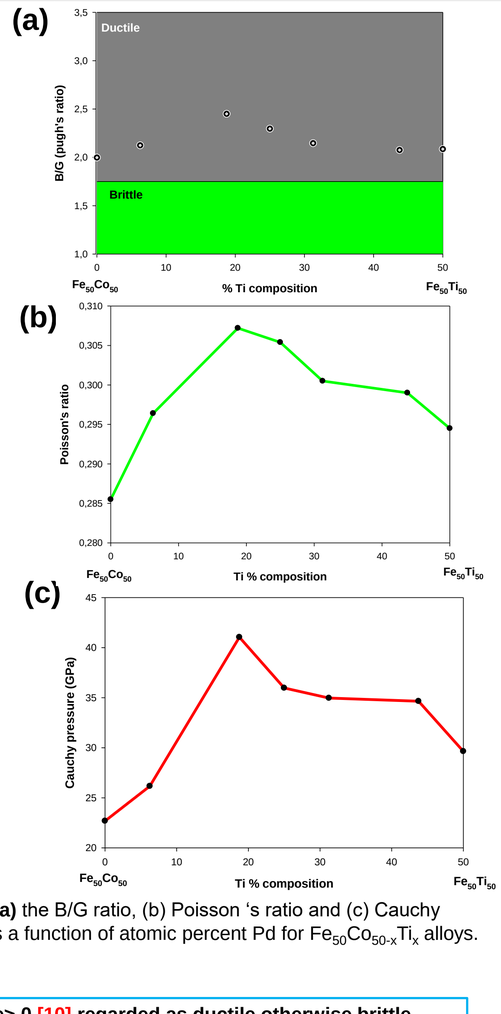


Figure. 4 **(a)** the B/G ratio, (b) Poisson 's ratio and (c) Cauchy pressure as a function of atomic percent Pd for $Fe_{50}Co_{50-x}Ti_x$ alloys.

The Pugh (B/G) > 1.75 [8], Poisson (σ)> 0.26 [9] and Cauchy pressure> 0 [10] regarded as ductile otherwise brittle.

In **Figure. 4 (a),** the B/G> 1.75 for the entire concentration range indicating ductile behaviour.

In **Figure, 4 (b) and (c)**, the σ and Cauchy pressure is greater than 0.26 and 0, respectively for the entire concentrations (0< x <50) (condition of ductility).

Figure. 5 show that $Fe_{50}Co_{50-x}Ti_x$ alloys have higher magnetic moments at 6.25 at. % Ti revealing that the structure has got higher magnetic strength.

Phonon Dispersion Curves

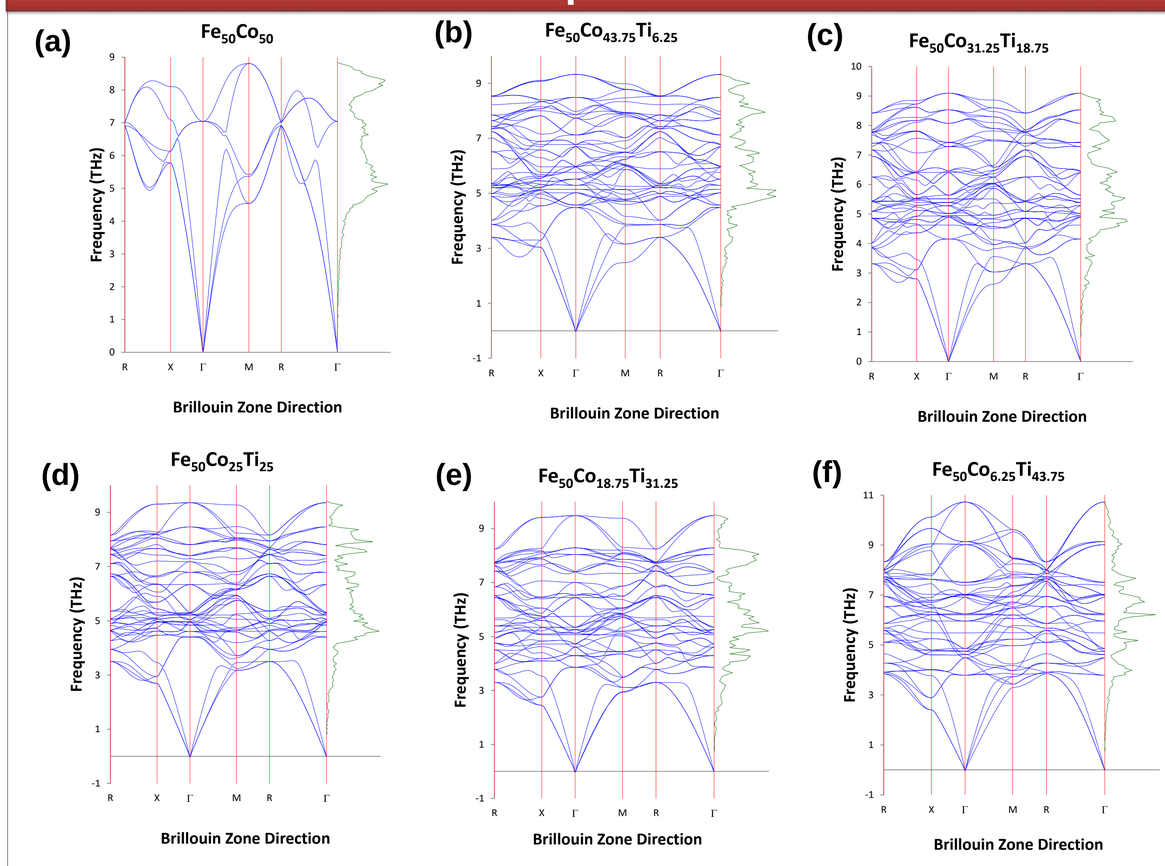


Figure. 6 (a-f) Phonon dispersion curves of the $Fe_{50}Co_{50-x}Ti_x$ ($0 \leq x \leq 43.75$) ternary structures

The phonon dispersion curves for the entire concentration range shows no negative vibrational frequencies suggesting that the materials are vibrational stable. These correspond with their positive shear moduli (*C'*).

Conclusions

The DFT approach was successfully used to study structural, thermodynamic, elastic and magnetic properties of B2 $Fe_{50}Co_{50-x}Ti_x$ structures for potential aerospace application. The results showed that $Fe_{50}Co_{50-x}Ti_x$ are thermodynamically stable with lowest heats of formation. The elastic properties were calculated and suggest that $Fe_{50}Co_{50-x}Ti_x$ structures are stable in agreement with the phonon dispersion curves. The B/G, Poisson 's ratio and Cauchy pressure showed a ductile manner for the entire composition where $0 \leq x \leq 50$. The findings suggest that ternary alloying with Ti enhances the ductility of the $Fe_{50}Co_{50}$ systems, and these alloys could be used in the development of future shape memory magnets for aerospace application.

References

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Acknowledgments

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