Computational studies of structural, mechanical and magnetic properties of the B2-phase $Fe_{50}Co_{50-x}Cr_x$ magnetic alloys

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Abstract. The B2 FeCo alloy is of great interest for high-temperature applications in the automotive industry as actuators due to its high saturation magnetization and Curie temperature. However, this alloy suffers from low ductility at room temperature. In this study, density functional theory applying the supercell approach was used to investigate the mechanical and magnetic properties of B2 $Fe_{50}Co_{50-X}Cr_X$ ($0 \leq x \leq 50$) structures. The stability of $Fe_{50}Co_{50-X}Cr_X$ was evaluated from the heats of formation, magnetic properties, and phonon dispersion curves. The heats of formation showed that doping with Cr enhances the thermodynamic stability of FeCo. Furthermore, the calculated Pugh and Poisson's ratios revealed that doping with Cr effectively enhances the ductility of FeCo. Thus, the results suggest that the B2 $Fe_{50}Co_{50-X}Cr_X$ alloy can be used for the future development of magnetic components with good strength in the automotive industry.

1 Introduction

FeCo alloys are widely known as soft magnetic materials (SMMs) [1]. These are materials that can be magnetized and demagnetized with ease, even in the existence of very little excitation field [2], resulting in high permeability. High saturation magnetization, low coercivity, high Curie temperature, and low power loss are the most important properties of soft magnetic materials, aside from their high reliability, low cost, and suitability for mass production, just like other commercial products [3]. The alloys are known as SMMs to contrast with hard magnetic materials (HMMs) which are used for permanent magnets [4]. Transformers, motors, inductors and generators use SMMs in their magnetic cores [5]. Commercially available soft magnetic alloys include FeNi, FeSi and FeCo [3]. Available SMMs are easy to break meaning they are less ductile or brittle. To improve the ductility, attempts were carried out previously to reduce the brittle nature and refine the ductility of Fe-Co alloys by ternary addition [14,15].

Previously, M.Matsuda et al probed the enhancement of ductility in FeCo-based alloys by substitution of Pd [18]. The experimental results revealed that 10 at. % Pd caused an increase in the ductility and tensile strength of FeCo. However, no information was given on how the ternary addition affects the magnetic properties of the alloy.

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Chromium (Cr) is the main anti-corrosive ingredient in stainless steel, and it is often used in alloys to increase strength and corrosion resistance. Therefore, the study aims to explore ways of enhancing the ductility of B2 Fe-Co at room temperature through ternary alloying with Cr using density functional theory. The ductility of $Fe_{50}Co_{50-x}Cr_x$ alloys is evaluated from Pugh and Poisson's ratios. Furthermore, the effect of Cr ternary addition on the structural, mechanical and magnetic properties of the alloy is determined.

2 Methodology

The density functional theory (DFT) [6,7] employing the Vienna ab initio simulation package (VASP) code [8] was used, together with the projector augmented wave (PAW) pseudopotential [9]. All calculations were performed considering the generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional [10]. To accomplish a convenient convergence of the parameters, an energy cut-off of 500 eV and k-spacing of 0.2 1/Å (12X12X12) were used according to Monkhorst and Pack [11]. From a 2x2x2 supercell structure of B2 $Fe_{50}Co_{50}$, different compositions (6.25, 18.75, 25, 31.25 and 43.75 at. % Cr) were generated. The structures were entirely relaxed in terms of volume, shape, and internal atomic locations until the atomic forces dropped below 0.01 eV/Å. The phonon dispersion curves of binary and ternary systems were determined using a PHONON code [12].

3 Results and discussion

3.1 Structural and thermodynamic properties

The ground-state properties of the ternary $Fe_{50}Co_{50-x}Cr_x$ alloys are shown in figure 1. The lattice parameters were determined from fully relaxed structures; both the lattice geometry and ionic positions were fully optimized. It was found that the lattice parameter of FeCo is 2.844 Å (2.843 Å [19]) which compares well with the experimental value in parenthesis to within 0.04 % agreement. The equilibrium lattice parameter of the $Fe_{50}Co_{50-x}Cr_x$ is observed to decrease as Cr content is increased (see figure 1). This effect may be attributed to the small atomic radius of Cr (128 pm) compared to Co (200 pm). The thermodynamic stability of $Fe_{50}Co_{50-x}Cr_x$ is argued through the predicted heats of formation (ΔH_f) and can be estimated by:

$$\Delta H_f(ab) = \frac{1}{N}[E_{Tot} - (E_a + E_b + \cdots)] \quad (1)$$

where N is the total number of atoms in the system, E_{Tot} is the calculated total energy of the compound while Ea and E_b are the enery of elements a and b. For a structure to be stable, the heat of formation must have a negative value ($\Delta H_f < 0$) otherwise a positive value implies instability. In Figure 2, we show the heats of formation for the B2 $Fe_{50}Co_{50-x}Cr_x$ systems for concentrations $0 \leq x \leq 50$. The heats of formation (ΔH_f) decreases below 6.25 at. % Cr, this implies that the structure becomes thermodynamically stable at this composition. Above 6.25 at. % Cr, it is observed that the heats of formation increase with an increase in Cr content. This suggests that thermodynamic stability is not enhanced by Cr addition when $18.75 \leq x \leq 50$ due to positive heats of formation ($\Delta H_f > 0$).

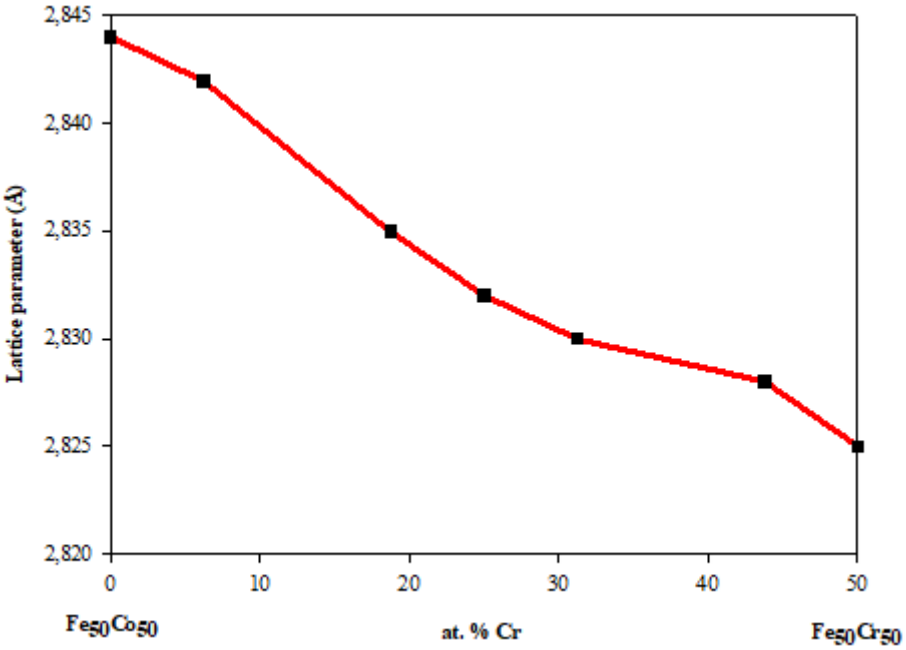


Fig. 1 Lattice parameter (Å) against atomic percent Cr for $Fe_{50}Co_{50-X}Cr_X$ alloys ($0 \leq x \leq 50$).

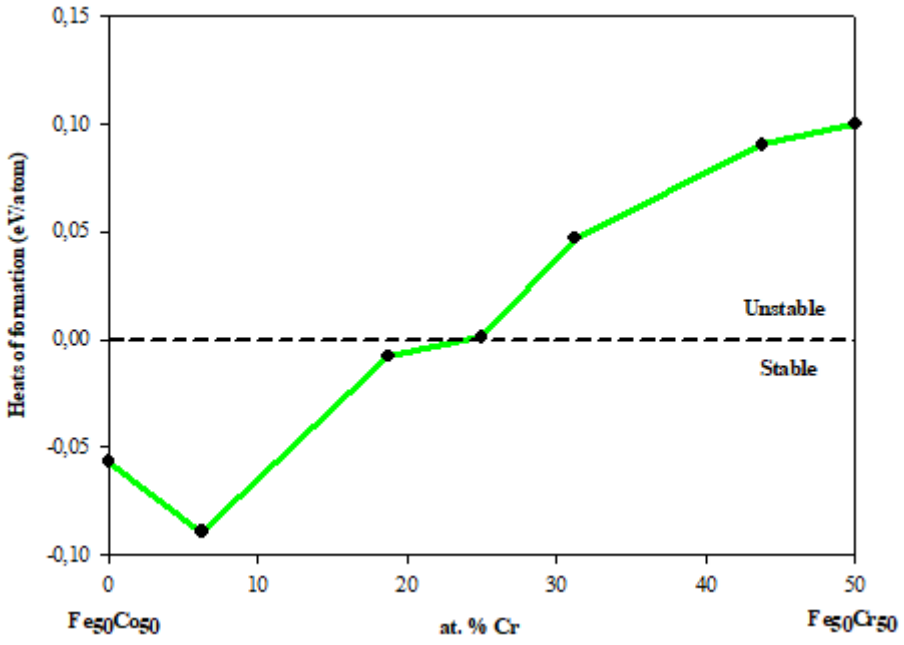


Fig. 2 Heats of formation, ΔH_f against atomic percent Cr for $Fe_{50}Co_{50-X}Cr_X$ alloys ($0 \leq x \leq 50$).

3.2 Magnetic properties

To probe into the magnetic strength of both binary $Fe_{50}Co_{50}$ and ternary $Fe_{50}Co_{50-x}Cr_x$ systems, the total magnetic moments were calculated. 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 3 shows the total magnetic moments of $Fe_{50}Co_{50-x}Cr_x$ alloys as a function of Cr atomic composition. 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 (4.479 μB) from literature [13]. The total magnetic moments decrease with an increase in Cr composition. This suggests that the magnetic strength of $Fe_{50}Co_{50}$ alloy is not enhanced with Cr addition.

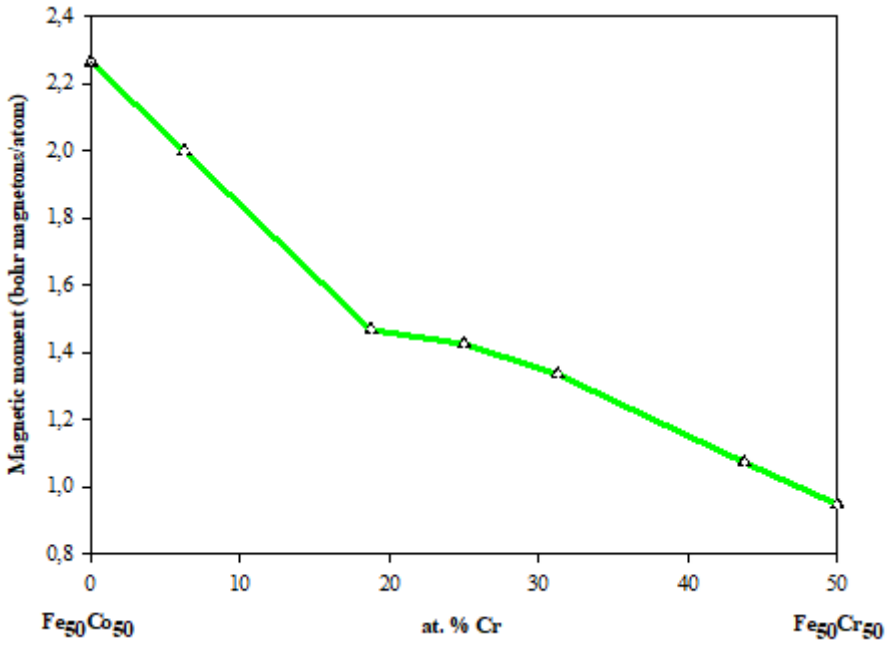


Fig. 3 Total magnetic moments against atomic percent Cr for $Fe_{50}Co_{50-x}Cr_X$ alloys ($0 \leq x \leq 50$).

3.3 Ductility

To measure the ductility of the materials, we have calculated the Poisson's ratios and Pugh (B/G) as shown in Figures 4 and 5, respectively. According to Poisson‘s ratio (σ), a structure is considered ductile when σ is greater than 0.26 otherwise brittle [16]. The Poisson’s ratio for FeCo was found to be 0.286 (0.290 [19]) which agrees with the theoretical value to within 1 %, implying that the material is ductile. As the content of Cr is increased, the σ values were found to be greater than 0.26 for all concentrations, condition of ductility (see figure 4). Note that a structure is considered ductile if the B/G ratio is greater than 1.75 and otherwise brittle as noted elsewhere [17]. It is seen that the B/G ratio for the binary FeCo was found to be 1.998 (B/G>1.75), condition of ductility. Likewise, the ductility increases as at. % Cr increases as shown in Figure 5. At 43.75 at. % Cr, ductility is the highest with the B/G value of 4.025.

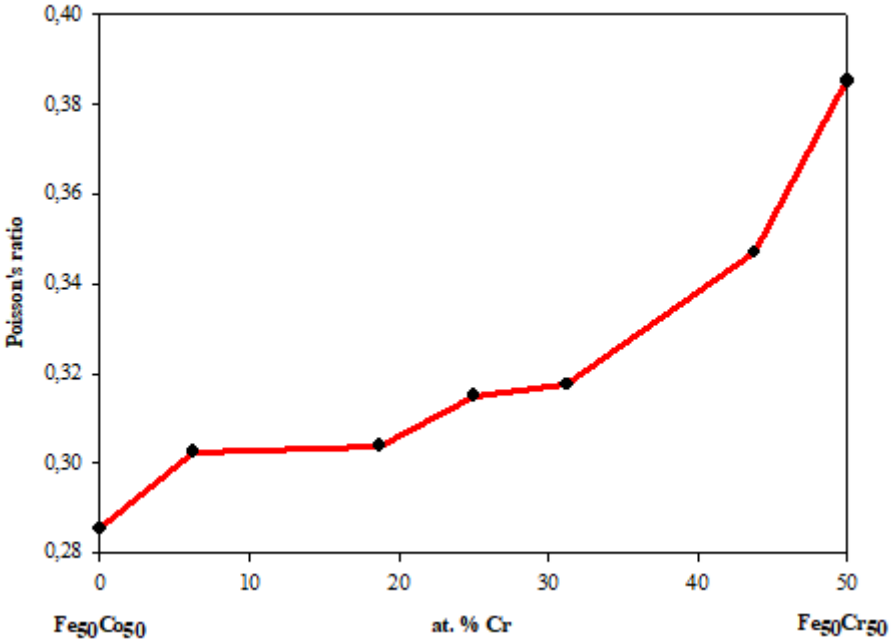


Fig. 4 Poisson's ratio against atomic percent Cr for $Fe_{50}Co_{50-x}Cr_x$, where $0 \leq x \leq 50$.

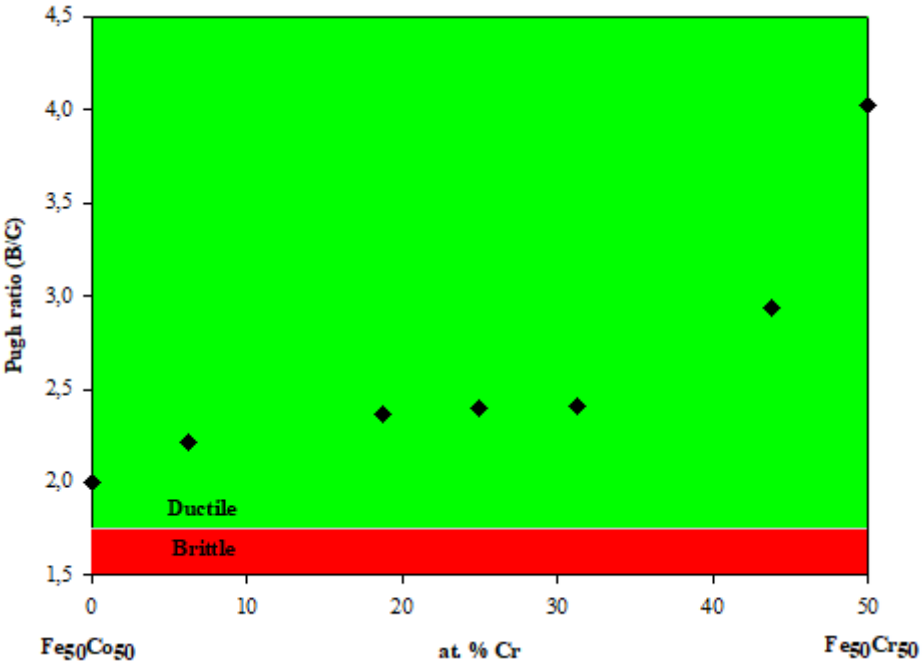
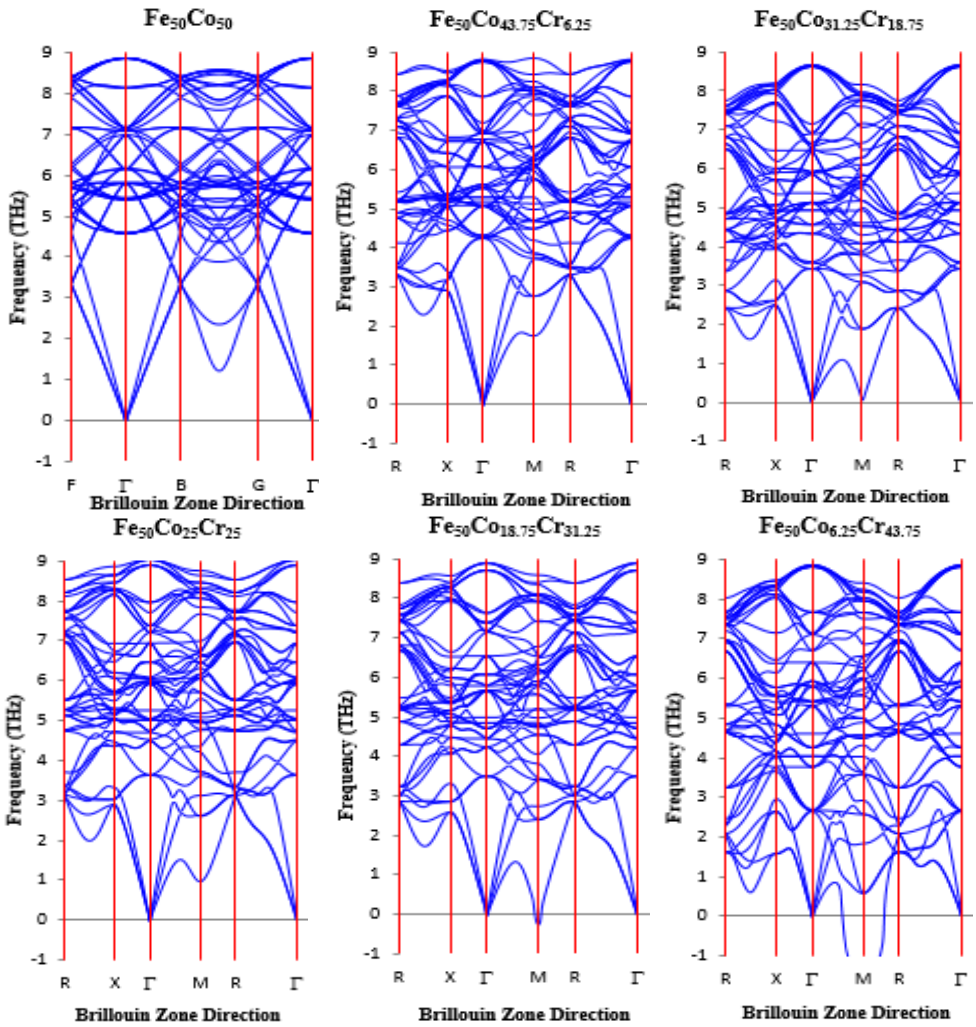


Fig. 5 Pugh ratio (B/G) against atomic percent Cr for $Fe_{50}Co_{50-x}Cr_x$, where $0 \leq x \leq 50$.

3.4 Phonon dispersion curves

The Phonon dispersion curves were calculated to determine the vibrational stability of B2 $Fe_{50}Co_{50-x}Cr_x$ alloys and are illustrated in figure 6. A structure is considered vibrationally stable if there are no soft modes along with negative directions in the Brillouin zone. It is noted that the phonon dispersion curves of B2 $Fe_{50}Co_{50-x}Cr_x$ are vibrationally stable for the entire concentration range ($0 \leq x \leq 50$) due to the absence of soft modes (i.e., positive frequencies). However, $Fe_{50}Co_{6.25}Cr_{43.75}$ display negative vibrations along M directions which do not imply mechanical instability rather it shows imaginary soft modes. This observation suggests that Cr addition does not compromise the stability of the B2 $Fe_{50}Co_{50}$ structure, and this is consistent with ductility predictions shown in Figures 4 and 5.



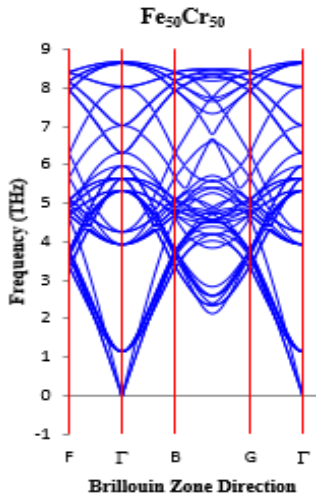


Fig. 6 Phonon dispersion curves for B2 $Fe_{50}Co_{50-x}Cr_x$ alloys.

Conclusion

The density functional theory method was successfully used to study the stability, ductility and magnetism of binary $Fe_{50}Co_{50}$ and ternary $Fe_{50}Co_{50-x}Cr_x$ systems. The lattice parameter of the B2 $Fe_{50}Co_{50}$ was found to fairly agree with previous experimental and theoretical data to within 0.04 %. It was revealed that a smaller concentration of Cr (<6.25 at. %) is required to improve the thermodynamic stability of B2 $Fe_{50}Co_{50}$, otherwise, the thermodynamic stability reduces at higher compositions. Furthermore, it was found that the calculated magnetic moment of the binary $Fe_{50}Co_{50}$ alloy agrees very well with that of previous theoretical work to within 1.14 %. In the case of ternary alloying, it was noted that alloying with Cr compromised the magnetism of B2 $Fe_{50}Co_{50}$. This study revealed that Cr has the potential to improve the ductility of the B2 FeCo alloy. The findings suggest that $Fe_{50}Co_{50-x}Cr_x$ alloys with small Cr composition (<10) can be used for the future development of magnetic components with good strength.

Acknowledgments

The authors wish to thank the financial support from the Titanium Centre of Competence (TiCoC) and the South African Research Chair Initiative of the Department of Science and Innovation (DSI). The computing resources offered by the Materials Modelling Centre (MMC) at the University of Limpopo and the Center for High-Performance Computing (CHPC) is highly appreciated.

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