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Ti CONTENT ON THE MAGNETIC AND MECHANICAL PROPERTIES OF B2 FeCo ALLOY: A COMPUTATIONAL STUDY

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, they suffer brittleness at room temperature. In this study, ternary alloying was used to investigate the strength of the alloys. Titanium was chosen as the alloying element since it has the potential to enhance the ductility of the alloy system. A density functional theory applying the supercell approach was used to investigate B2 Fe50Co50-XTiX ($0 \leq X \leq 50$) structures. A full optimization was performed and provided equilibrium ground-state properties for both binary and ternary systems. It was found that the equilibrium lattice parameters are in good agreement with the experiment to within 2%. The stability of Fe50Co50-XTiX was evaluated from the formation energies, elastic properties, magnetic properties, and phonon dispersion curves. It was found that the thermodynamic stability increased with an increase in Ti content as observed from the heats of formation. Furthermore, the calculated Pugh's and Poisson's ratios showed that alloying with Ti effectively enhances ductility. Moreover, Fe50Co50-XTiX systems showed positive shear modulus for the entire concentration range, a condition of stability. This observation accord well with the phonon dispersion curves analysis. Thus, the results suggest that the B2 FeCo-Ti alloy can be used for the development of magnetic components with good strength, that can be used for actuator applications.

Apply to be considered for a student ; award (Yes / No)?

Yes

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MSc

Primary authors: Prof. CHAUKE, Hasani (University of Limpopo); Prof. NGOEPE, Phuti (University of Limpopo); Mrs DIALE, Ramogohlo (University of Limpopo); Ms LEDWABA, Tebogo (University of Limpopo)

Presenter: Ms LEDWABA, Tebogo (University of Limpopo)

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