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Structural and magnetic properties of Mn50Pt50-xNix alloys: A first principles study

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L10 MnPt alloy has attracted much attention recently since it can be easily produced and provides magnetic properties of interest to spintronic applications. According to previous studies, this alloy retains its anti-ferromagnetism at room temperature. In this study, a first-principles calculations were performed in the framework of density functional theory to identify new spintronic material compositions in Mn-based alloys. By using this method, the structural, electronic structure, thermodynamic, elastic and magnetic properties were determined to track the stability of Mn50Pt50-xNix (x=0, 6.25, 12.5, 18.75, 25) alloys. It was found that the calculated lattice constants of binary systems are in good agreement with available experimental data. According to heats of formation calculations, B2 and L10 Mn50Pt50-xNix alloys are thermodynamically stable when c/a is less than 1.10 suggesting that these alloys can be synthesized experimentally. Furthermore, it was found that the magnetic moments improve with an increase in Ni compositions when the c/a ratio is 1.10 and drops above (c/a>1.10). As a result of these findings, more guided experimental studies can be undertaken on promising Mn50Pt50-xNix alloys for potential use in future spintronic devices.

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

No

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Primary author: Dr DIALE, Ramogohlo (MINTEK)

Co-authors: Prof. NGOEPE, Phuti (University of Limpopo); Dr PHASHA, Maje (MINTEK); Mr MOEMA, Joseph (MINTEK); Prof. CHAUKE, Hasani (University of Limpopo)

Presenter: Dr DIALE, Ramogohlo (MINTEK)

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