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The effect of ferromagnetic elements (Fe, Ni) on the magnetic properties of MnPt alloy

The L10 MnPt alloy is useful for magnetic recording and spintronic applications due to its high ferromagnetic stability. Previous studies showed that this alloy maintains its ferromagnetism at room temperature. In this study, first-principles method was used to investigate the effect of partial substitution of Mn in MnPt with ferromagnetic elements M (M= Fe, Ni). The ground-state properties of the binary Mn₅₀Pt₅₀ are found to agree with the available experimental data and others theoretical results. The heats of formation of L10 Pt₅₀Mn_{50-x}M_x alloys were found to be negative, suggesting that the alloys are thermodynamically possible to form. Furthermore, L10 Pt₅₀Mn_{43.75}M_{6.25} was predicted to be the most stable structure (displaying the lowest heats of formation) when the c/a ratio is 1.11 compared to other competing ratios. A ferromagnetic state can be attained in Pt₅₀Mn_{50-x}M_x by a small difference in the tetragonality ratio from 1.1 to 1.3. The elastic constants, Bulk, Shear and Young's moduli were also calculated. Finally, the ductility of Pt₅₀Mn_{50-x}M_x was evaluated using the B/G ratio, Cauchy pressure and Poisson's ratio σ . As a result, a first-principles method was successfully used to understand the magnetism and stability of Pt₅₀Mn_{50-x}M_x alloys upon introduction of ferromagnetic Fe and Ni.

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

No

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N/A

Primary author: Dr DIALE, Ramogohlo (UL and MINTEK)

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

Presenter: Dr DIALE, Ramogohlo (UL and MINTEK)

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