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The effect of Ir on the magnetic and electronic properties of FePt alloy: A DFT study

L1₀-ordered FePt alloy is a promising material for high-density magnetic recording media due to its high magnetic anisotropy energy, density and coercivity. However, it was reported that this alloy faces challenges including issues with thermal stability and noise. Hence, ternary alloying with Ir was conducted to enhance the stability in response to the orientation of the magnetic spin moment of the binary FePt system. The structural, magnetic electronic and thermal properties of L1₀-ordered Fe₅₀Pt_{50-x}Ir_x alloys (0≤x≤25) were studied using the Density Functional Theory. It was found that the lattice parameters and magnetic moments of the binary Fe₅₀Pt₅₀ are well in agreement with previous theoretical and experimental data to within 5 %. In all Fe₅₀Pt_{50-x}Ir_x alloys, the calculated heats of formation were negative, demonstrating their thermodynamic stability. The magnetic moments and density of states were determined to evaluate the magnetic behaviour of Fe50Pt50-xIrx alloys. These results contribute to the development of Fe₅₀Pt_{50-x}Ir_x alloys as the next generation of magnets for high-density magnetic recording media.

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Primary authors: MATLALA, Mashilo (University of Limpopo); MATSHABA, Malili (University of Limpopo); CHAUKE, Hasani Richard (University of Limpopo); DIALE, Ramogohlo (Mintek)

Presenter: MATLALA, Mashilo (University of Limpopo)

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