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Enhancement of the magnetic and mechanical performance of L10 MnPt-Ru alloys using ab initio techniques

The rapid advancement of high-performance computing and spintronic technologies demands the development of novel materials that combine high magnetic anisotropy, thermal stability, and mechanical robustness. $L1_0$ ordered MnPt is a promising rare-earth-free candidate due to its large magnetocrystalline anisotropy and strong spin polarization. However, its practical application is hindered by brittleness, mechanical instability and phase segregation at elevated temperatures. In this study, we investigate the impact of Ru on the structural, thermodynamic, electronic, magnetic, and mechanical properties of $L1_0$ MnPt alloy using first-principles calculations. The lattice parameters and magnetic moments of binary $L1_0$-ordered MnPt alloy agree well with experimental and theoretical data to within 5 %. Heats of formation , elastic constants and thermophysical properties were determined to check the stability of L 10 Mn50Pt50-xRux alloys ($0 \leq x \leq 25$). The findings will contribute to the design of high-performance MnPt-based alloys, providing a pathway toward rare-earth-free magnetic materials with improved thermal and mechanical performance.

Keywords: Mn50Pt50-xRux alloys, DFT, Magnetic strength, Mechanical properties

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