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Density functional theory study on the effect of pressure on structural, mechanical and electronic properties of A15 M3Ru alloy

Ruthenium-based alloys exhibit strong potential for aerospace applications. This study employs first-principles DFT calculations to examine the impact of pressure on the structural, electronic, mechanical, and phonon properties of Mn_3Ru in its A15 crystallographic phase. At zero pressure, Mn_3Ru has a negative formation energy of -0.64 eV, indicating thermodynamic stability. However, as the pressure increases from 50–200 GPa, the heat of formation becomes slightly positive, hence compromising its stability at equilibrium conditions. The density of states reveals a transition from half-metallic to metallic behavior under pressure. The alloy is mechanically unstable at 0 and 50 GPa due to negative C_{44} values but stabilizes at elevated pressures of between 100–200 GPa. Phonon dispersion confirms dynamic stability across all pressure ranges. This study demonstrates that while the application of pressure may marginally reduce the thermodynamic stability of Mn_3Ru, it significantly improves its mechanical and dynamic properties, thereby making it a promising alloy for high-temperature structural application.

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