Contribution ID: **74** Type: **Oral Presentation**

Exploring the structural, magnetic, and elastic properties of Mn50Al50-xSnx alloys: A DFT study

Tuesday 8 July 2025 10:50 (20 minutes)

Permanent magnets have the unique property of maintaining a high magnetic flux density when there is no external magnetic field. The ferromagnetic τ-phase MnAl intermetallic compound stands out as a promising candidate for rare earth-free magnets, attributed to its good machinability, low cost, and low density. However, the material was reported to be brittle and thermodynamically unstable. To mitigate this problem, the density functional theory is employed to investigate the structural, thermodynamic, magnetic, and elastic properties of Mn50Al50-xSnx alloys in the range (0≤x≤25). The lattice parameters of the binary MnAl were found to be in good agreement with previous theoretical and experimental data within 5%. Heats of formation results showed that substituting Al with Sn slightly decreases the thermodynamic stability of Mn50Al50-xSnx alloys. It was found that Mn50Al50-xSnx, in the range (0 ≤ x ≤ 25), shows ferromagnetic behavior due to non-zero net spin magnetic moments. Doping with Sn was found to enhance the magnetic strength of the system. The brittleness of the system reduces with increasing Sn concentration; however, complete ductility is not yet attained. The findings will provide valuable insights into the development of advanced permanent magnets.

Keywords: Mn50Al50-xSnx alloys, Density Functional Theory (DFT), Magnetic properties, Ductility

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Session Classification: Physics of Condensed Matter and Materials 2

Track Classification: Track A - Physics of Condensed Matter and Materials