Phase Transitions and Magnetic Properties of Transition Metal Based Magnetocaloric Materials

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\*\*\*General Introduction\*\*\*

This dataset contains data collected during magnetocaloric materials synthesis and experiments at Delft University of Technology, as part of Hanggai's PhD Thesis project (June 2025): doi: 10.4233/uuid:07e1fac3-ae48-4677-8557-693bbb6bbe64. It is being made public both to act as supplementary data for publications and the PhD thesis of Hanggai and in order for other researchers to use this data in their own work.

The data in this dataset was collected in the Fundamental Aspects of Materials and Energy Laboratory of the Delft University of Technology - Faculty of Applied Science, between Dec. 2020 and December 2024. This research project was made possible by a grant from the Dutch Research Council (NOW).

\*\*\*Purpose of the test campaign\*\*\*

The purpose of these experiments was to investigate the structure, microstructure, and magnetic properties of novel (Mn,Fe)3Sn magnetocaloric materials for potential application in magnetic heat pumps. Magnetization measurements were conducted to determine the transition temperature and saturation magnetization. Neutron diffraction measurements for investigating the spin structure of this type of materials. Mössbauer measurements for investigating the spin reorientation. DFT calculations preformed for investigate the local magnetic moments for specific elements Mn and Fe.

\*\*\*Test equipment\*\*\*

All magnetic measurements were performed using a Superconducting Quantum Interference Device (SQUID). Temperature-dependent scans were conducted under applied magnetic fields of 0.01 T and 1 T, while field-dependent scans were carried out at 5 K with magnetic fields ranging from 0 to 5 T. Neutron diffraction measurements performed at RID TU Delft. The transmission 57Fe Mössbauer spectra were collected at different temperatures with a conventional constant-acceleration spectrometer using a 57Co(Rh) source. Velocity calibration was carried out using an *α*-Fe foil at room temperature. The Mössbauer spectra were fitted using the Mosswinn 4.0 program. Density functional theory (DFT) calculations were carried out with the Vienna *ab initio* simulation package (VASP) using the Perdew-Burke-Ernzerhof (PBE) exchange correlation functional and the PAW method.

\*\*\*Description of the data in this data set\*\*\*

The data included in this data set has been organised per specimen. The files follow the nomenclature system: XRD diffraction data with X = angle Y = cont. per second. Magnetization data with X = temperature (K), Y =magnetization (emu). Neutron data with X = angle Y = cont. per second. DFT data with X = energy Y = density of state.