INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: Study of Magnetocaloric Effect in Off-stoichiometric Ni-Mn-Sb Heusler Compounds by Density Functional Theory and Monte Carlo Methods

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SHORT ABSTRACT

Solid-state cooling or heating using magnetocaloric materials has emerged as an energy efficient green technology. The magnetocaloric effect (MCE) describes the thermal response of a magnetic material due to the application of a magnetic field which is quantified by isothermal magnetic entropy change (ΔS_{mag}) and the adiabatic temperature change (ΔT_{ad}). An extended search of new magnetocaloric materials exhibiting giant MCE, in an appropriate temperature range, as well as improving performances of the existing ones, is an active area of current research. Among different types of magnetocaloric materials, Ni-Mn based magnetic shape memory Heusler alloys are of great interest since they exhibit giant MCE associated with the first-order magneto-structural transition. In this thesis, we have investigated the Ni-Mn-Sb based Heusler systems where significant magnetocaloric effects are observed near room temperature. Our investigation focused on off-stoichiometric Ni-Mn-Sb and Fe, Co and Cu substituted Mn-excess Ni-Mn-Sb compounds. We investigated the impact of various factors, such as composition, site occupancy, magnetic structure, magnetic interactions on structural phase stability, transition temperatures, mechanical properties, and consequently the magnetocaloric parameters of compounds in Ni-Mn-Sb family. We have done first-principles Density Functional Theory (DFT) calculations in conjunction with Monte Carlo simulation method using model Hamiltonians which incorporated the magnetic, structural and magneto-structural degrees of freedom. We have developed a Monte Carlo simulation code and used the Heisenberg model, the BEG model and the q-state Potts model for computations of magnetocaloric parameters near a first-order magneto-structural transition and a second-order magnetic transition in substitutional Ni-Mn-Sb compounds. Our calculations reproduced the experimental results on systems where experiments were done and also predicted a few new compounds in the family that can exhibit significantly large magnetocaloric effect, near room temperature. In essence, the results presented in this thesis on Ni-Mn-Sb based Heusler compounds, on one hand, provides a protocol for identifying materials potentially useful for magnetocaloric applications, using results of DFT calculations and on the other hand, quantifies the magnetocaloric effects in those materials, thus paving ways for experimentalists to design new magnetocaloric materials.