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Magneto

Caloric Effect in Ni-Mn-Ga alloys: First Principles and Experimental studies KHORGOLKHUU ODBADRAKH, DON NICHOLSON, Oak Ridge National Laboratory, GREGORY BROWN, Florida State University, AURELIAN RUSANU, ORLANDO RIOS, JASON HODGES, ATHENA SAFA-SEFAT, GERARD LUDTKA, MARKUS EISENBACH, BOYD EVANS, Oak Ridge National Laboratory — Understanding the Magneto-Caloric Effect (MCE) in alloys with real technological potential is important to the development of viable MCE based products. We report results of computational and experimental investigation of a candidate MCE materials Ni-Mn-Ga alloys. The Wang-Landau statistical method is used in tandem with Locally Self-consistent Multiple Scattering (LSMS) method to explore magnetic states of the system. A classical Heisenberg Hamiltonian is parametrized based on these states and used in obtaining the density of magnetic states. The Currie temperature, isothermal entropy change, and adiabatic temperature change are then calculated from the density of states. Experiments to observe the structural and magnetic phase transformations were performed at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL) on alloys of Ni-Mn-Ga and Fe-Ni-Mn-Ga-Cu. Data from the observations are discussed in comparison with the computational studies. This work was sponsored by the Laboratory Directed Research and Development Program (ORNL), by the Mathematical, Information, and Computational Sciences Division; Office of Advanced Scientific Computing Research (US DOE), and by the Materials Sciences and Engineering Division; Office of Basic Energy Sciences (US DOE).

Khorgolkhuu Odbadrakh
Oak Ridge National Laboratory

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