MM 34: Topical session: Caloric effects in ferroic materials IV - Heuslers

Time: Wednesday 11:45–12:45 Location: H39

MM 34.1 Wed 11:45 H39

Nucleation barrier of martensite in magnetocaloric Heusler films — •Robert Niemann[1,2], Anett Diestel[1], Anja Backen[1], Sandra Hahn[3], Martin F.-X. Wagner[3], Ludwig Schultz[1,2], and Sebastian Fähler[1,2] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Technische Universität Dresden, Department of Physics, Institute for Solid State Physics, D-01062 Dresden, Germany — [3]Technische Universität Chemnitz, Institute of Materials Science and Engineering, D-09107 Chemnitz, Germany

Martensitic transformations in magnetic shape memory alloys lead to large temperature- and field-dependence of the magnetization and accordingly to large entropy changes. These ferroic materials are discussed for applications in solid-state cooling cycles, but only if the thermal hysteresis can be reduced. Therefore it is important to understand the origin of hysteresis and to differentiate the contributions of nucleation and growth. As a model system we study epitaxial thin films of Heusler alloy Ni-Mn-Ga-(Co). The shape of the nucleus is known from in-situ experiments. We calculate the theoretical barrier for homogeneous nucleation using a continuum model of the nucleus and employing classical nucleation theory. From time-dependence of the magnetization we can identify growth and nucleation events and calculate the respective energy barriers. The energy necessary for nucleation is also derived from the difference between full and minor loops of the transformation. We conclude that only heterogeneous nucleation is possible and show that the barrier is effectively reduced by nanoindentation. Funded by DFG SPP1599 www.FerroicCooling.de

MM 34.2 Wed 12:15 H39

Impact of point defects on the phase stability in Heusler alloys: A first-principles study — •Biswanath Dutta, Vijaya Begum, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Functional properties of magnetic Heusler alloys such as magnetic shape memory and magnetocaloric effect depend critically on their thermoelastic martensitic transformation. To this end, vacancies can play a decisive role as they control the ordering kinetics in these materials, which has recently been confirmed in experiments. Within this study, we employ density functional theory along with Monte Carlo (MC) simulations to understand the impact of vacancies on the phase stability and transformation behavior in Ni-Mn-based Heusler alloys. Our calculations reveal high vacancy concentrations for Ni and Mn with the vacancy formation energy for Ni being the lowest. We discuss the results in terms of chemical potentials obtained against the formation of different unary and binary phases. The nudged elastic band method is employed to compute the vacancy migration barrier. Our calculated results for the self-diffusion activation energy of vacancies show good agreement with experimental values. Using these results as input for MC simulations we discuss the impact of vacancies on the ordering tendency in these materials.

MM 34.3 Wed 12:30 H39

Magnetocaloric and microstructural properties of Half-Heusler-type alloys — •Andreas Taubel, Tino Gottschall, Konstantin P. Skokov, Iliya A. Radulov, and Oliver Gutfleisch — Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

Magnetocaloric refrigeration offers an efficient and environmentally friendly alternative to conventional gas compression cooling. Besides the well-known Gd-Si-Ge and La-Fe-Si systems, Heusler alloys and their related Half-Heusler and MM′X materials come into focus. The Mn-Ni-Ge system exhibits a martensitic phase transition from its high temperature hexagonal phase to its low temperature orthorhombic phase with a broadly tunable transition temperature when partially substituting Fe for Mn or Ni. Previous studies already showed a sharp transition with low hysteresis and considerable changes in magnetization during the transition. In this work, we could obtain very large isothermal entropy changes ΔS_m of up to -37.8 $Jkg^{-1}K^{-1}$ based on magnetic measurements of small single pieces. However the high volume change of 2.7 % results in an embrittlement of large particles into several smaller grains. For this reason bonding of the material with a polymer epoxy was carried out in order to enable direct measurements of ΔT_{ad} and to evaluate the possibility for its usage under real conditions in a magnetocaloric cooling device.

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