Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

First principles determination of phase transitions in magnetic shape memory alloys[1] TILMANN HICKEL, MPI fuer Eisenforschung GmbH, MATTHE UIJTTEWAAL, JOERG NEUGEBAUER — Magnetic shape memory alloys have recently attracted a lot of excitement, since they allow shape changes of more then 10% with a frequency in the kHz regime. The fundamental origin of this property is related to a martensitic phase transition. The material system Ni_2MnGa is the most promising candidate for applications, but its operation temperatures and ductility still need to be improved. Hence, an extension of the currently very limited knowledge on the phase diagram is decisive. In order to identify the stable structures and their transitions we performed ab initio calculations of free energies for the austenite, the (modulated) pre-martensite and the unmodulated martensite. Quasiharmonic phonons and fixed-spin magnons are considered, employing density functional theory. Using this approach we were able to successfully describe the phase transition in detail, to reveal the involved delicate interplay of vibrational and magnetic excitations and to accurately determine the transition temperature. The methods are used to interpret the experimental findings and to make predictions for modified material compositions.

[1]Financial support of DFG via SPP1239 is gratefully acknowledged.

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Date submitted: 19 Nov 2008 Electronic form version 1.4