Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Origin of magnetic interactions and their influence on the structural properties of Ni2MnGa and related compounds BURAK HIMMETOGLU, MATTEO COCOCCIONI, University of Minnesota — In this work, we perform first principles DFT calculations to investigate the interplay between magnetic and structural properties in Ni_2MnGa. We demonstrate that the relative stability of austenite (cubic) and non-modulated martensite (tetragonal) phases depend critically on magnetic interactions between Mn atoms. While standard approximate DFT functionals stabilize the latter phase, a more accurate treatment of electronic localization and magnetism obtained with DFT+U suppresses the non-modulated tetragonal structure for the stoichiometric compound, in better agreement with the experiments. This observation can be explained using the Anderson impurity model, where Mn atoms are treated as periodic magnetic impurities embedded in Ga p and Ni d conduction electrons that mediate RKKY type magnetic interactions between Mn d electrons. Using this picture we show that the structural properties of the material are determined by the competition between super-exchange interactions mediated through Ni d and Ga p states. Finally, we show that off-stoichiometric compositions with excess Mn promote transition to a non-modulated tetragonal structure, in agreement with experiments.

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Date submitted: 26 Oct 2011 Electronic form version 1.4