Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Element specific analysis of magnetic anisotropy in practical Mn-based antiferromagnetic alloys from first principles KHMELEVSKYI SERGII, Institute of Applied Physics, Vienna University of Technology, Austria, ALEXANDR B. SHICK[1], Institute of Physics ASCR, v.v.i., Na Slovance 2, 182 21 Praha 8, Czech Republic, PETER MOHN, Institute of Applied Physics, Vienna University of Technology, Austria — Magnetic Anisotropy Energy (MAE) and element specific contribution to MAE has been studied for practical Mn-based antiferromagnetic alloys with layered $L1_0$ structure in the framework of the Local Spin Density Approximation and fully relativistic torque method. It is found that the contribution to the total MAE from non-magnetic 3d and 4d-elements in MnNi and MnPd alloys is comparable to the contribution of the magnetic Mn atoms. In the 3d-5d MnIr alloy the Ir contribution is found to be dominating. The origin of this contribution from the elements with total zero atomic spin moment is linked to the calculated non-trivial spin density distributions on the corresponding atom, which gives a zero moment only on average. We have also found and discuss a strong dependence of the total and element specific contribution to MAE on the state of the magnetic order.

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Date submitted: 22 Dec 2010 Electronic form version 1.4