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, 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 L10 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.

1shick@fzu.cz

Sergii Khmelevskyi
Institute of Applied Physics, Vienna University of Technology

Date submitted: 22 Dec 2010