Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Stacking-fault energy and anti-Invar effect in FeMn alloys at high temperature ANDREI REYES-HUAMANTINCO[1], PETER PUSCHNIG, CLAUDIA AMBROSCH-DRAXL, Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria, OLEG PEIL, I. Institute for Theoretical Physics, Hamburg University, Germany, ANDREI RUBAN, Applied Material Physics, Royal Institute of Technology, Stockholm, Sweden — High-Mn steels (20-30at%Mn, 2-4wt%Si and Al) are of interest for the automotive industry due to their outstanding mechanical properties. Their deformation behavior has been empirically correlated to the stacking-fault energy (SFE), an important quantity in steel design that can be calculated *ab-initio*. Using state-of-the-art methods within density-functional theory together with Monte Carlo simulations, we calculate the free energy of the Fe-22.5at%Mn binary alloy between 300-800 K. Experimentally, the alloy is completely random and in the paramagnetic state, which we model via the coherent potential approximation and the disordered local moment approach, respectively. We treat magnetic excitations by including longitudinal spin-fluctuations and find that the FeMn alloy is an itinerant paramagnet. Our calculations confirm the experimentally observed strong magneto-volume coupling, realized in the anti-Invar behavior. We then obtain the structural stability and the SFE from free energy differences and find very good agreement with measurements. Our results demonstrate that the interplay between magnetic excitations and the thermal lattice expansion is the main factor determining the anti-Invar effect, the *fcc-hcp* martensitic transformation temperature and the SFE.

[1]Second Affiliation: Materials Center Leoben, Austria

Andrei Reyes-Huamantinco
Chair of Atomistic Modelling and Design of Materials,
University of Leoben, Austria

Date submitted: 18 Nov 2011 Electronic form version 1.4