

Abstract Submitted  
for the MAR13 Meeting of  
The American Physical Society

**Magnetic anisotropy of strained MnGa alloys** RENAT SABIRIANOV, NABIL AL-AQTASH, University of Nebraska at Omaha — MnGa is a promising candidate for Rare Earth free permanent magnet applications because it has a large magnetocrystalline anisotropy. We examine the variation of the magnetocrystalline anisotropy of these alloys as function of bi-axial in-plane strain using ab-initio electronic structure calculations. We employed force theorem to calculate the MAE= $E(\parallel)$ - $E(\perp)$  as difference of energies of the system with magnetization along and perpendicular to the easy axis. Using projector augmented wave method implemented in VASP we have calculated MAE in MnGa, Mn<sub>3</sub>Ga and Mn<sub>1+x</sub>Ga<sub>1-x</sub> alloys. We find that the MAE is 2.5MJ/m<sup>3</sup> (0.42meV/u.c.) and 0.12MJ/m<sup>3</sup> (0.07meV/u.c.) in unstrained MnGa and Mn<sub>3</sub>Ga, respectively. MAE decreases if bi-axial strain is applied in MnGa. Thus, the anisotropy of this system can be affected by the strain. We also discuss the effect of Mn disorder on MAE in Mn<sub>1+x</sub>Ga<sub>1-x</sub> alloys.

Renat Sabirianov  
University of Nebraska at Omaha

Date submitted: 17 Nov 2012

Electronic form version 1.4