Origin and tuning of the magnetic anisotropy in Fe$_2$P-based alloys

IVAN ZHURAVLEV, Department of Physics and Astronomy, University of Nebraska-Lincoln, V.P. ANTROPOV, Ames Laboratory, U.S. Department of Energy, Ames, Iowa 50011, USA, K. D. BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska-Lincoln — Fe$_2$P-based alloys have been studied for years due to their potential magnetocaloric applications. In addition, Fe$_2$P demonstrates record-high magnetocrystalline anisotropy (MCA) for systems with no heavy elements. While the Curie temperature $T_C$ in pure Fe$_2$P is too low for applications, this system appears to be highly tunable, and its $T_C$ can be greatly increased by alloying with many other $d$ and $p$ elements. Here we present the electronic structure analysis of magnetic properties of these alloys, searching for systems with higher $T_C$ while preserving high MCA. The microscopic origin of the dominant contribution to MCA and its concentration dependence is revealed. We further find that co-alloying with Co or Ni and Si is a promising strategy for achieving high Curie temperature and MCA, which is more favorable compared to individual alloying by Co/Ni or Si due to the compensation of their effects on the band occupation.

$^1$Work at UNL supported by NSF Grants DMR-1308751 and DMR-1609776. Work at Ames Lab was supported by the Critical Materials Institute, an Energy Innovation Hub funded by the US DOE.

Ivan Zhuravlev
Department of Physics and Astronomy, University of Nebraska-Lincoln

Date submitted: 11 Nov 2016 Electronic form version 1.4