Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Calculated magnetic structure of mobile defects in Fe[1] DON NICHOLSON, KH. ODBADRAKH, GERMAN SAMOLYUK, G. MALCOLM STOCKS, Oak Ridge National Lab — Mobile defects such as dislocations and crowdions respond to gradients of strain, temperature, concentration, and applied field, thereby, determining a material's viability in particular applications. In Fe, defects affect the magnetic state of the surrounding atoms. We discuss the defect-induced changes in magnetic moment magnitude and orientation, magnetic anisotropy and magnetic interactions. These quantities are calculated (density functional theory (DFT)) for defect models ranging in size from a few hundred to a few thousand. Comparisons are made between different DFT methods. The importance of magnetism to the response of defects to gradients is discussed.

[1]This work was supported by the Center for Defect Physics, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.

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Date submitted: 12 Dec 2012 Electronic form version 1.4