Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Investigation of electronic and magnetic properties of wurtzite NiO thin films[1] BRIAN BUSEMEYER, Department of Physics, University of California, Davis, CA 95616-8677 USA, MICHAEL SHAUGHNESSY, Sandia National Laboratories at Livermore, Livermore, CA 94551 USA, LIAM DAMEWOOD, C.Y. FONG, Department of Physics, University of California, Davis, CA 95616-8677 USA — We study the electronic and magnetic properties of wurtzite (B4) NiO thin films grown epitaxially on wide gap semiconductors to understand factors affecting their half-metallic properties, in particular, the effect of film thickness, interface geometry, and dangling bonds. One, two, and four consecutive layers of NiO are considered, both buried within bulk ZnO, and as thin surface films on bulk ZnO. We perform GGA+U calculations, with the U value determined via a self consistent linear response approach. We find that the interface generates small s-p hybridized states at the Fermi energy, which can possibly destroy the half metallicity; these states are likely due to effects from strain at the interface. We also find that the interface can influence the Ni d states in markedly different ways, depending on the geometry and the presence of dangling bonds. These factors can determine whether the interface Ni d states resemble those from Ni in bulk wurtzite NiO, or demonstrate semiconductivity, more akin to d states of Zn atoms within bulk ZnO.

[1]Work at UC Davis was supported in part by the National Science Foundation Grant No. ECCS-1232275.

Brian Busemeyer
Department of Physics, University of California,
Davis, CA 95616-8677 USA

Date submitted: 19 Nov 2012 Electronic form version 1.4