Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

The atomic and electronic structure of the FeCoB/MgO interface J.D. BURTON, S.S. JASWAL, E.Y. TSYMBAL, University of Nebraska Lincoln, O.N. MRYASOV, O.G. HEINONEN, Seagate Technology — Magnetic tunnel junctions (MTJs) have recently aroused much interest due to their potential applications as random access memories and magnetic field sensors. MTJs consist of a thin insulating layer separating two ferromagnetic electrodes. Very recently FeCoB/MgO/FeCoB MTJs have shown promising results. Upon annealing, the amorphous FeCoB electrodes crystallize in a bcc structure epitaxial to the MgO(001) surface. Many groups have observed a significant increase in TMR ratios (higher than 300% at room temperature [1]) after annealing. It is clear that the crystallization of the electrodes plays an important role in this increase. It is not clear, however, what happens to B after annealing and what role it plays in enhancing TMR. We present results of first-principles total energy calculations that suggest that it is energetically favorable for B to reside at the crystalline FeCoB/MgO interface rather than remain in the bulk of the FeCoB electrode. We also find that the presence of B at the interface significantly weakens bonding between the FeCoB electrode and the MgO barrier. We are investigating the presence of resonant states[2] at the FeCoB/MgO interface and will discuss the effects of interfacial B on them. [1] J. Hayakawa *et al.*, 2005 MMM Conference. [2] Belashchenko *et al.*, *Phys. Rev. B* **72**, R140404 (2005).

J. D. Burton

Date submitted: 02 Dec 2005 Electronic form version 1.4