Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Oxygen-Induced Reconstructions on the $\beta-\mathbf{Si_3N_4}$ $(10\bar{1}0)$ Surfaces WERONIKA WALKOSZ, JUAN CARLOS IDROBO, SERDAR OGUT[1], University of Illinois at Chicago — Motivated by recent electron microscopy studies at the Si_3N_4/rare-earth oxide (REO) interfaces, we present first principles calculations for the preferred bonding sites and configurations of oxygen on various terminations of the $\beta-Si_3N_4$ $(10\bar{1}0)$ surface as a function of coverage and surface stoichiometry. We predict that oxygen induces various surface reconstructions, and it has a strong tendency to replace N on the surface. The structural stability of most low-energy surfaces is driven by the tendency of Si to saturate its dangling bonds and of oxygen to bridge two Si atoms similar to the bonding in SiO_2. The present *ab initio* results resolve the discrepancy between the experimental observations at the Si_3N_4/REO interfaces and previous theoretical studies[2] for bare surfaces regarding the lowest energy surface termination.

[1]Supported by NSF Grant No. DMR-0604964
[2]Juan C. Idrobo *et al.*, Phys. Rev. B **72**, 241301(R) (2005).

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Date submitted: 27 Nov 2007 Electronic form version 1.4