

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**Atomic and Electronic Structures of Oxygen on the  $\beta$ -Si<sub>3</sub>N<sub>4</sub> (10 $\bar{1}$ 0) Surface**<sup>1</sup> WERONIKA WALKOSZ, JUAN C. IDROBO, SERDAR OGUT, University of Illinois at Chicago — The desirable mechanical and physical properties of Si<sub>3</sub>N<sub>4</sub> ceramics in high temperature applications are hindered by their intrinsic brittleness. Doping Si<sub>3</sub>N<sub>4</sub> with rare-earth oxides has long been known to overcome this limitation creating a tougher material. Precise information about the microscopic origin of this empirical observation has, however, been lacking for many years. In this study, we present *ab initio* calculations for the structural stability of  $\beta$ -Si<sub>3</sub>N<sub>4</sub> (10 $\bar{1}$ 0) surfaces in the presence of different oxygen concentrations. Two different (10 $\bar{1}$ 0) surface terminations, the “open ring” and the “half surface”,<sup>2</sup> are investigated in detail using an asymmetric slab. We find that the Si-O bond plays the most important role in the structural stability and passivation of the surface. The theoretical results are analyzed in connection with recent electron microscopy studies on the interface.<sup>3</sup>

<sup>1</sup>Work supported by NSF Grant No. DMR-0605964

<sup>2</sup>J. C. Idrobo *et al.*, Phys. Rev. B **72**, 241301(R) (2005).

<sup>3</sup>A. Ziegler *et al.*, Science **306**, 1768 (2004); N. Shibata *et al.*, Nature **428**, 730 (2004); G. B. Winkelmann *et al.*, Phil. Mag. Lett. **84**, 755 (2004).

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Date submitted: 20 Nov 2006

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