Abstract Submitted
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Atomic and Electronic Structures of Oxygen on the $\beta-\mathbf{Si_3N_4}$ $(10\bar{1}0)$ Surface[1] WERONIKA WALKOSZ, JUAN C. IDROBO, SERDAR OGUT, University of Illinois at Chicago — The desirable mechanical and physical properties of Si_3N_4 ceramics in high temperature applications are hindered by their intrinsic brittleness. Doping Si_3N_4 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 $\beta-Si_3N_4$ $(10\bar{1}0)$ surfaces in the presence of different oxygen concentrations. Two different $(10\bar{1}0)$ surface terminations, the "open ring" and the "half surface",[2] 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.[3]

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[2]J. C. Idrobo *et al.*, Phys. Rev. B **72**, 241301(R) (2005).
[3]A. Ziegler *et al.*, Science **306**, 1768 (2004); N. Shibata *et al.*, Nature **428**, 730 (2004); G. B. Winkelman *et al.*, Phil. Mag. Lett. **84**, 755 (2004).

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