

Abstract Submitted  
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**Film Growth and Surface Energy of (100) CrO<sub>2</sub>** HUNTER SIMS, KRISHNA CHETRY, MAIRBEK CHSHIEV, MINT Center and Department of Physics, University of Alabama, ARUNAVA GUPTA, MINT Center and Department of Chemistry, University of Alabama, WILLIAM BUTLER, MINT Center and Department of Physics, University of Alabama — Rutile structure CrO<sub>2</sub> can be grown epitaxially on a rutile TiO<sub>2</sub> substrate. Surprisingly, growth in the (100) direction is layer by layer even though surface energies evaluated using the VASP code [1] indicate that the surface energy of TiO<sub>2</sub> is less than the sum of the surface energy of CrO<sub>2</sub> and the CrO<sub>2</sub>-TiO<sub>2</sub> interface energy[2]. It is known however, that CrO<sub>2</sub> (100) surfaces spontaneously decompose to form an epitaxial Cr<sub>2</sub>O<sub>3</sub> phase. We have investigated the conjecture that the layer by layer growth of CrO<sub>2</sub> results from the formation of a surface layer substoichiometric in oxygen. If the conjectured substoichiometric layer forms, it must be converted to CrO<sub>2</sub> as it is covered. We calculate the energy of a (100) fully stoichiometric surface, a (100) surface with oxygen removed, and a (100) surface with an interior oxygen deficiency using the standard relaxation methods in the VASP code as well as its simulated annealing capabilities. By comparing the energies (taking into account the removed oxygen in the latter two cases), we can predict the behavior of the CrO<sub>2</sub> films during deposition.

[1] G. Kresse and J. Hafner, Phys. Rev. B 47, 558 (1993); G. Kresse and J. Hafner, Phys. Rev. B 49, 14 251 (1994).

[2] K. Chetry and A. Gupta, unpublished

Hunter Sims  
MINT Center and Department of Physics, University of Alabama

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