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Variation of Growth Mode with Orientation for Epitaxial CrO_2 Films KRISHNA CHETRY, HUNTER SIMS, WILLIAM BUTLER, ARUN GUPTA, University of Alabama — Thin films of CrO_2 have been grown epitaxially on (110) and (100) oriented TiO_2 substrates. CrO_2(100) films grow in a layer by layer mode, while an island growth mode is observed for CrO_2(110) films as confirmed from atomic force microscopy (AFM) studies. To better understand the differences in the growth mode, we have performed first principles-based calculations using density functional theory implemented within the VASP code to study the surface and interface energies of CrO_2 (100), (110), TiO_2 (100) and (110) systems. For these calculations a periodic repeating slab geometry is used with a sufficient vacuum width and thickness to converge the surface energy within $0.01 J/m^{-2}$ From our calculations we find that in case of (110) orientation $\sigma_{TiO_2} > \sigma_{CrO_2} + \gamma$, where σ is the surface energy and γ is the interface energy between CrO_2 and TiO_2 system. This result is consistent with the island growth mode observed experimentally for (110) orientation. For the case of (110) orientation also we find that $\sigma_{TiO_2} < \sigma_{CrO_2} + \gamma$, which does not match with our experimental results. We speculate that formation of some oxygen deficient phase of chromium oxide in the very first monolayer, which then gets converted to CrO_2 by accepting oxygen from the second layer, favors the layer-by-layer growth mode in CrO_2 (100).

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