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Ferromagnetism in Co doped anatase TiO_2 thin films mediated by Co-Ti^{+3}-V_O complexes MARIA VARELA, Oak Ridge National Lab, KELLI GRIFFIN-ROBERTS, University of Washington, SERGEY RASHKEEV, Idaho National Lab, SOKRATES PANTELIDES, Vanderbilt University, STEPHEN PENNYCOOK, Oak Ridge National Lab, KANNAN KRISHNAN, University of Washington — The correction of spherical aberration in the STEM has enabled sub-Angstrom imaging and spectroscopy, and, in favorable cases, direct imaging of light atoms and interstitials. We identify the origin of ferromagnetism in $Co_{0,03}$:TiO_2 anatase thin films by combining STEM, EELS and DFT calculations. The films are insulating and ferromagnetic at room temperature. Ferromagnetism is enhanced by a post growth vacuum annealing suggesting a defect-mediated mechanism in these films. DFT finds interstitial Co to be energetically preferred over substitutional Co. STEM imaging reveals the interstitials in the predicted sites, and EELS finds reduced Ti in adjacent columns, also predicted by DFT. The combination of STEM-EELS-DFT therefore identifies the defect responsible for the magnetism: an O vacancy binds to the interstitial Co to form a Co-Ti^{+3}-V_O complex, with a magnetic moment in good agreement with the observed value. Research sponsored by Div. of Materials Sciences and Engineering US DOE, and NSF/ECS 0224138.

Maria Varela
Oak Ridge National Lab

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