

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Ta doped TiO₂: substitutionality and bandgap variation A. ROY BARMAN, S. DHAR, M. MOTAPOTHULA, T.K. CHAN, M. BREESE, G. OS-IPOWICZ, T. VENKATESAN, NanoCore, National University of Singapore, Singapore 117576, NANOCORE, NATIONAL UNIVERSITY OF SINGAPORE, SINGAPORE 117576 TEAM — We report on the growth of high quality single crystal anatase Ta_xTi_{1-x}O₂ films on (001) LaAlO₃ substrate by Pulsed Laser Deposition at various substrate temperatures, O₂ partial pressures, and Ta concentrations. We use X-Ray diffraction and Rutherford backscattering-ion channeling experiments to study the epitaxial film growth and Ta substitutionality. Ta is found to be almost completely substituted in the Ti sites resulting in the expansion of the TiO₂ lattice constant with Ta concentration. A strong oxygen pressure and temperature dependence of the Ta substitution is also noticed. The bandgap of the doped TiO₂, measured by UV-Vis spectroscopy, shows a blue shift. This appears to be more consistent with the formation of an alloy Ta_xTi_{1-x}O₂ with a bandgap given by a linear combination of the bandgaps of the TiO₂ and Ta₂O₅, in accordance with the Vegard's law rather than the band filling effects (Moss-Burstein shift). The origin of this blue shift will be presented and discussed along with the experimental results.

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Date submitted: 02 Dec 2009

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