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Scaling of Flat Band Potential and Dielectric Constant as a Function of Ta Concentration in Ta-TiO2 Epitaxial Films[1] Y.L. ZHAO, A. ROY BARMAN, S. DHAR, A. ANNADI, NUSNNI-NanoCore, NUS, M. MOTAPOTHULA, CIBA,NUS, J.H. WANG, H.B. SU, Material science, NTU, M. BREESE, CIBA,NUS, T. VENKATESAN, NUSNNI-NanoCore, NUS, Q. WANG, Material science, NUS — Electrochemical impedance spectroscopy measurements of pulsed laser deposited single crystal anatase TiO2 thin films with various concentrations of Ta substituting for Ti were carried out. UV-visible measurements show a systematic increase of the bandgap with Ta incorporation. Corresponding Mott-Schottky plot was applied to obtain a continuous shift of the flat band potential with increasing free charge carrier concentration. This was verified theoretically by ab initio calculation which shows that extra Ta d-electrons occupy Ti t2g orbital with increasing Ta concentration, thereby pushing up the Fermi level. The Mott-Schottky results were consistent when compared with Hall effect and temperature dependent resistivity measurements. From the measured deviation of carrier densities from Hall and Mott-Schottky measurements we have estimated the static dielectric constant of the TiO2 as a function of Ta incorporation. We are able to estimate the shifts of both the conduction and valence bands from these measurements.

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