A design study of TiO_2/n-Si energy band structure for charge carrier transportation in water splitting electrode

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Introduction: The present work aims to design a semiconductor system for an effective charger carrier separation and transportation process in a water splitting electrode. Therefore, a conduction band discontinuity between anatase phase titanium dioxide (A-TiO_2) and n-type silicon (n-Si) was investigated in this study. A-TiO_2 for the survey of a junction between TiO_2 and Si was deposited on an n-Si substrate via a spin-coating technique followed by a two-step annealing process. Three different n-type Si substrates with dopant density of $10^{15\text{-}16}$; $10^{17\text{-}18}$; $10^{20\text{-}21}$ cm^{-3} were used in this study. XRD and FE-SEM techniques were used for crystal phase and surface microstructure analysis. Electronic states of TiO_2 and n-Si for energy band evaluation was measured with XPS. Current-Voltage characteristics and dark-current were measured for a better understanding of charge carrier transfer in the TiO_2/n-Si junction.

According to the energy band gap of TiO_2 (E_g = 3.5 eV) and n-Si (E_g = 1.12 eV) together with valence band maximum (VBM) and valence band offset (VBO) evaluated regarding XPS analysis, and conduction band minimum (CBM) with conduction band offset (CBO) which was calculated based on previous analysis, a concept diagram was designed for the TiO_2/n-Si system (Fig. 1). The CBO for TiO_2/n-Si is $CBO_{(TiO2/n\text{-}Si)}$ = -0.12 eV, with CBM of TiO_2 at lower energy level than that of n-Si. Depletion layer for the TiO_2/n-Si junction depends on n-Si dopant density and changes from 361-1140 nm ($10^{15\text{-}16}$ cm^{-3}) to 1.14 – 3.61 nm ($10^{20\text{-}21}$ cm^{-3}). Thus, having a low doped n-Si substrate, only charge transfer from n-Si to TiO_2 is possible. With increased dopant density, the depletion layer narrows and enables the tunneling effect which allows a current flow both directions without knee and breakdown voltage (ohmic contact). A broader explanation of the study will be explained in the presentation.

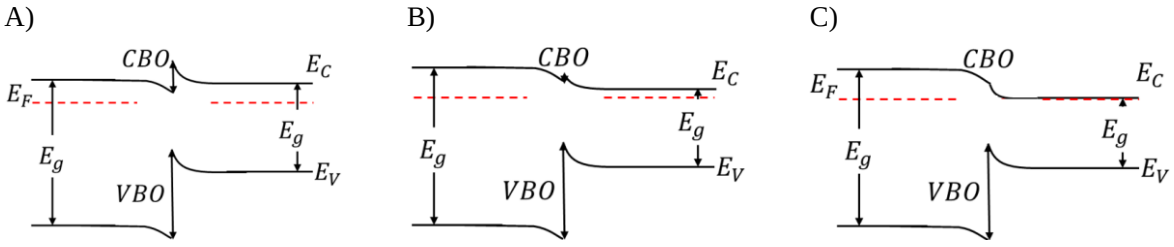

Fig. 1. Schematic models of the energy band alignment in n-type Si/TiO_2 heterojunction interface. A) N_D= $10^{15\text{-}16}$ cm^{-3}; B) N_D= $10^{17\text{-}18}$ cm^{-3}; C) N_D= $10^{20\text{-}21}$ cm^{-3}.

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