



Figure 15.2 Scanning electron microscope photograph of a typical nanocrystalline TiO_2 film: the scale bar corresponds to $0.43 \mu\text{m}$

900 nm. Absorption by these dyes in the visible and near-IR regions is attributed to the metal-to-ligand charge-transfer (MLCT) transition. The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are mainly derived from the d-orbitals of the Ru metal and the π^* orbital of the ligand, respectively. The NCS ligand shifts the HOMO level negatively, leading to a red shift in the absorption property of the complex, and also contributes electron acceptance from reduced redox ions (I^-). These Ru complexes have carboxyl groups to anchor to the TiO_2 surface. Anchoring causes a large electronic interaction between the ligand and the conduction band of TiO_2 , resulting in effective electron injection from the Ru complex into the TiO_2 . The Ru complex is adsorbed on the TiO_2 surface via either carboxylate bidentate coordination or ester bonding ($-\text{C}(=\text{O})\text{O}-$) as measured by FT-IR absorption analysis [19–23]. Figure 15.5 shows the anchoring structure of the N3 dye adsorbed on the (101) surface of TiO_2 . The coverage of the TiO_2 surface with the N3 dye reaches near 100% as derived from the surface area of TiO_2 and the amount of the dye.

15.1.2.4 Redox electrolyte

The electrolyte used in the DSSC contains I^-/I_3^- redox ions, which mediate electrons between the TiO_2 photoelectrode and the counter electrode. Mixtures of iodides such as