Lattice Mismatch along the Interface of Anatase and TiO_2(B) for Lithium Storage

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Titanium dioxide (TiO_2), one of the most promising anode materials for lithium-ion batteries, has been extensively studied, not only due to its low cost, abundance and non-toxicity but also on account of the negligible volume deformation during the Li-ion intercalation/de-intercalation processes and excellent gravimetric capacity. Charge stored in a Li^+/heterophase anode system may be enhanced through interfacial charge storage at both the solid-liquid interface and internal solid-solid interfaces. Jamnik and Maier[1,2] have demonstrated increased charge storage at TiO_2-metal interfaces as a result of the metal acting as an electron sink and the TiO_2 storing excess Li^+. In TiO_2 photochemical studies, it has been demonstrated that owing to the offset in the conduction band levels, photogenerated charge carriers can be stored at the junction between anatase and TiO_2(B). This band offset has been employed in TiO_2 engineering to yield a material in which Li^+ and electrons are separated across TiO_2(B)/anatase TiO_2 interfaces within the anode leading to increased charge storage[3].

In this work we have fabricated a new TiO_2-graphene composite designed to enhance the prospects of this low cost, abundant, non-toxic material as an anode in a Li-battery. The TiO_2 is dandelion shaped with nanosized TiO_2(B) fibrils capped with anatase TiO_2 pappi. Electronmicroscopy indicates that the composite contains triphase boundaries between anatase, TiO_2(B) and graphene, which are responsible for the enhancement of energy storage and the decrease of electrode polarization. Cyclic voltammetric investigations point to both Li^+ insertion and pseudocapacitative contributions to charge storage. Ultrahigh specific capacities of 243 and 182 mAh g^{-1} have been obtained at 0.1 and 1 A g^{-1}, respectively. Moreover, the excellent capacity retention can reach 99.6% after 100 cycles with almost 100% coulombic efficiency at 0.1 A g^{-1}.

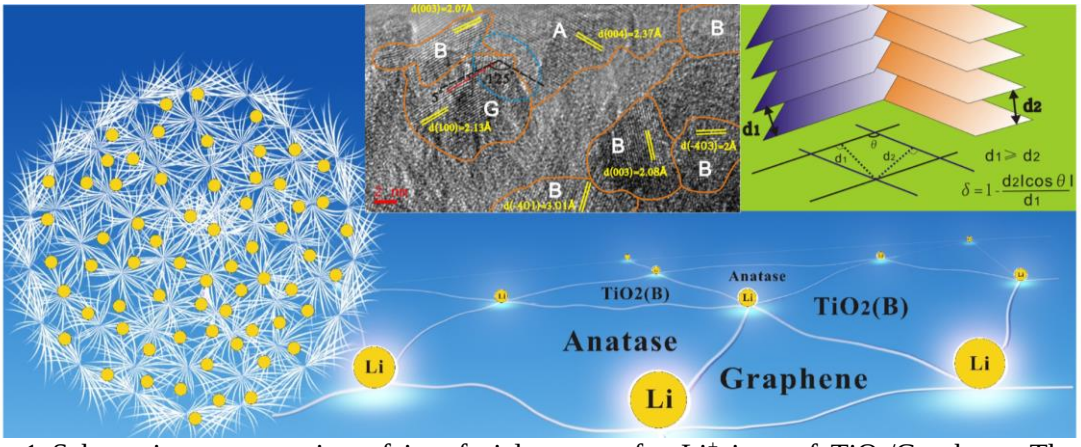

Figure 1 Schematic representation of interfacial storage for Li^+ ions of TiO_2/Graphene. The inset shows lattice mismatch between anatase and TiO_2(B) phases and the calculation of mismatch rate, δ.

References:

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[2] J. Jamnik and J. Maier, *Phys. Chem. Chem. Phys.*, 2003, 5, 5215.
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