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Investigation on Lithium Storage Properties of Solvothermal-synthesized Pyrite FeS₂ Nanocubes

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Lithium ion battery (LIB) is one of the most widely used forms of rechargeable batteries in today's consumer portable electronics, due mainly to its high energy density and good cycling performance. These properties, coupled with growing attention on renewable energies and environmental sustainability, have led to search for better battery materials that can increase the energy storage, improve the reliability and, yet, reduce the cost of LIBs. Iron sulfides have been used in the battery field for a long time, in particular as electrode material in thermal and lithium primary batteries due to its high theoretical capacity of 890 mAhg⁻¹, non-toxicity, earth abundance and low cost. However, iron sulfides are known to react irreversibly with lithium at ambient temperature, hence limiting its use in secondary LIBs. This work investigates the use of pyrite FeS₂ as electrode material for rechargeable LIB application. Nanostructuring of the material has been done to alleviate the problem of poor cycling performance and capacity retention of the FeS₂ electrode. Nanomaterials have a shorter lithium ion diffusion length than its bulk counterparts, thus giving better rate capability. Additionally, anode materials with unique morphologies have been chemically synthesized by different research groups and were demonstrated to exhibit better capacity retention. Therefore, in this work, pyrite FeS₂ nanocubes of about 100nm were synthesized using a simple, one-step solvothermal method. Time-dependent characterization was done to understand the formation mechanism of the nanocubes and it was found that the precursors first react to form sheet-like amorphous Fe_{1-x}S which upon further heating transforms into pyrite FeS₂ nanocubes. The lithium storage properties of the as-synthesized FeS₂ nanocubes are characterized and found to exhibit a stable cycling performance with a discharge capacity of 555mAhg⁻¹ after 50 charge/discharge cycles at a high current density of 1Ag⁻¹. Even at a higher current density of 5Ag⁻¹, the pyrite FeS₂ electrode still managed to achieve a stable discharge capacity of about 220mAhg⁻¹. Ex-situ analysis of the pyrite FeS₂ electrode charged and discharged for different cycles was done to investigate and understand the excellent performance exhibited by the pyrite FeS₂ nanocubes.

Keywords Lithium ion batteries; Solvothermal; FeS₂; Pyrite