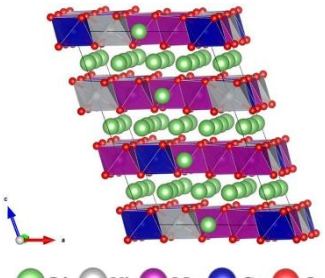
鋰離子電池高容量正負極材料與高穩定性電解液開發

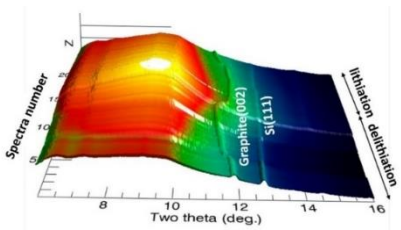
執行單位	國立成功大學材料科學及工程學系	計畫主持人	方冠榮教授

- 本計畫開發高容量正負極材料與高穩定性電解液之儲能元件技術。鋰離子電池是具高克電容量、高能量密度之高價值儲能元件，能廣泛應用在 3C、通訊、智慧電網與電動車輛。

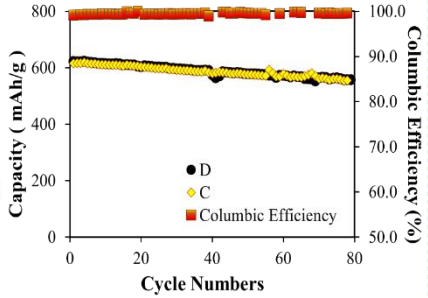
證書號：M513213
專利名稱：電化學反應及產氣收集裝置
本新型揭露一種電化學反應及產氣收集裝置，透過本發明之一種電化學反應及產氣收集裝置應用於電化學反應及產氣收集系統。於電化學反應進行時，藉由集氣罐體、及氣密管路接頭，在收集反應裝置充放電時所產生之氣體，進而對其分析。



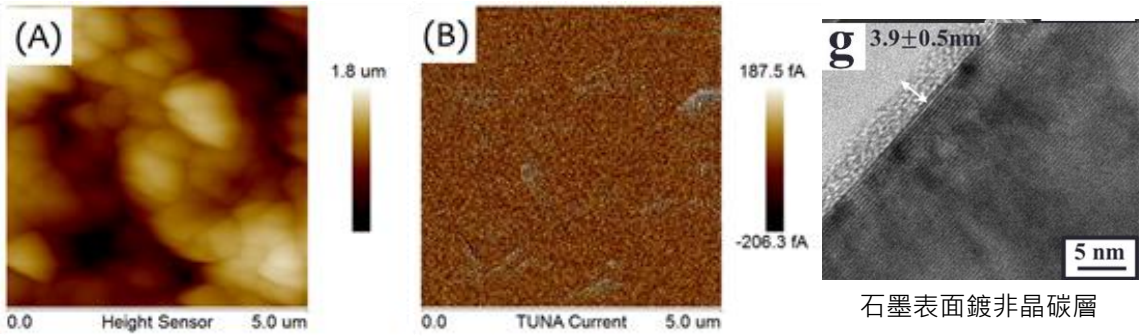
層狀正極材料之原子級模型



矽碳複合材料結構演繹



矽碳複合材料循環壽命



AFM分析
石墨表面鍍非晶碳層

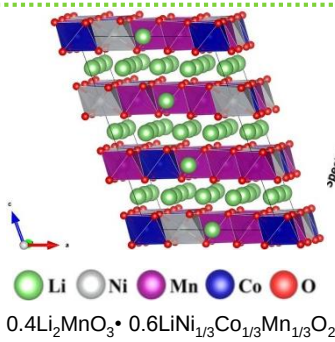
- 建構 $0.4Li_2MnO_3 \cdot 0.6LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$複合層狀正極材料之原子級模型。計算$Li_4Ti_5O_{12}$負極材料的摻雜之競爭相與反應能。
- 合成$0.5Li_2MnO_3$-$0.5LiMO_2$粉末製備、晶體結構與顯微結構分析。其電容量可達到269 mAh/g，30圈電池循環測試後仍可維持221 mAh/g。
- 完成添加劑分子的HOMO, LUMO, OP, RP分別在氣態以及溶液態的計算以及類神經網路的建立以及參數的設定。
- 矽材料首圈放電電容量2586 mAh/g、庫侖效率89.9%，循環充放電100圈後，電容量2149 mAh/g，維持率83%。矽碳材料首圈放電電容量610 mAh/g、庫侖效率91.6%，循環充放電80圈後，電容量555 mAh/g，維持率91%。
- 分析鋰金屬表面形貌與微結構，以及單極式探針應用於$Li_4Ti_5O_{12}$負極材料界面之阻抗量測。
- 利用含浸法/熱處理法將石墨材料表面控制鍍上可調整2-20 nm 的非晶碳層。石墨表面鍍上約4 nm左右的非晶碳層後，可以提升電容量約12%。
- 利用同步輻射臨場繞射技術觀察各式矽碳複合材料電性變異與結構演繹。

Development of anode, cathode and electrolyte material for high-capacity and stability lithium-ion battery application

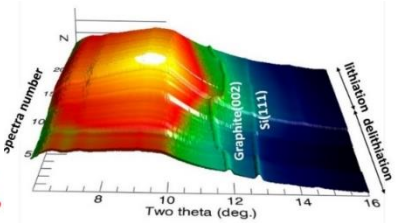
Execution Unit	Department of Materials Science and Engineering, National Cheng Kung University
Project Director	Professor Kuan-Zong Fung

- This project aims to develop high capacity cathode and anode materials and high stability electrolyte for lithium-ion batteries. Lithium-ion batteries have attracted significant attention for applications in portable electronics, power tools, hybrid/full electric vehicles, and energy storage system.

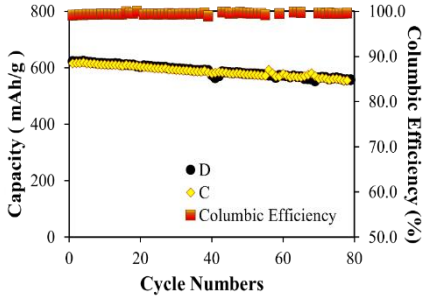
I518331：Conductive probe and insulating trenches manufacturing method thereof
The invention discloses a conductive probe and insulating trenches manufacturing method thereof. The conductive probe is applied in atomic force microscopy (AFM) and includes a base, a plurality of support elements, a plurality of tips and a conductive layer.



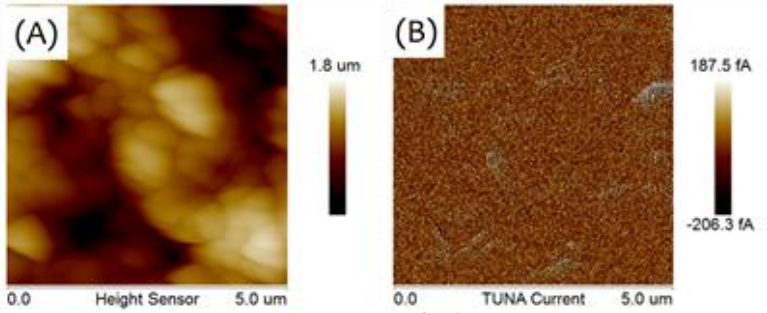
$0.4Li_2MnO_3 \cdot 0.6LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$



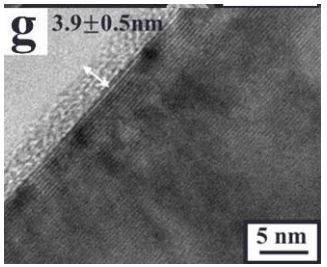
structure evolution of Si/C



Cycle life of Si/C



AFM analysis



An amorphous carbon layer on graphite

- The atomic structures of $0.4Li_2MnO_3 \cdot 0.6LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ and $Li_4Ti_5O_{12}$ were successfully modeling by first-principles calculation.
- The lithium-rich cathode material delivered a discharge capacity of 269 mAh/g and maintained a discharge capacity of 221 mAh/g after 30 cycles.
- By the first principle molecular dynamics calculation, the reduction of PS molecules is prior to that of EC molecules during the first charge, consequently suppresses the decomposition of EC and gas production.
- The discharge capacity of Si/C material was 610 mAh/g with the coulombic efficiency of 91.6% in the first cycle. The capacity decreased to 555 mAh/g with the capacity retention of 91% after 80 cycles.
- AFM micro-area measurement technology was used to effectively distinguish the surface properties of $Li_4Ti_5O_{12}$ materials.
- An amorphous carbon layer with 4 nm in thickness prepared by impregnation method followed by thermal treatment can increase the capacity of graphite by 12%.
- The crystal structure interaction between silicon and graphite with respect to Li intercalation and extraction was elucidated by using in-operando X-ray diffraction technique.