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Performance of NMC622 Cathode - LTO Anode Full Cell Lithium Ion Battery

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Abstract: At present, the demand for renewable energy sources is steadily increasing, and accordingly, the use of electric vehicles has become more widespread. This trend has led to a growing focus on the development of alternative anode and cathode materials. In this study, NMC622 ($LiNi_{0.6}Co_{0.2}Mn_{0.2}O_2$) with a layered structure was employed as the cathode, while spinel-structured LTO ($Li_4Ti_5O_{12}$), which holds the second-largest market share after graphite, was selected as the anode. The crystal structures of the prepared anode and cathode electrodes were characterized using X-ray diffraction (XRD). The electrochemical performance of the full cell was evaluated by assembling it into a CR2032-type coin cell. The full cell was initially activated at a rate of 0.1 C, after which galvanostatic charge/discharge tests were performed to assess its electrochemical performance at rates of 0.5 C, 1 C, 2 C, and 5 C over 100 cycles. The initial discharge capacities at 0.5 C, 1 C, 2 C, and 5 C were determined as 127, 120, 105, and 70 mA h g^{-1}, respectively. Across all C-rates, the capacity retention ratios were found to vary between 65% and 70%.

Keywords: NMC622, LTO, Li-ion batteries

Introduction

Today, a significant portion of the world's energy demand is met by fossil fuels, which have high carbon emissions. Fossil fuels are finite energy resources and contribute to global warming issues (Ahmad et. al., 2020; Kanoğlu et. al., 2019) Efforts to reduce the use of fossil fuels depend on increasing the use of renewable energy sources and the widespread adoption of electric vehicles. Lithium-ion (Li-ion) batteries, first introduced for commercial use by Japan's Sony Corporation in 1991, have become indispensable for electronic devices due to their high specific energy density and are excellent candidates for energy storage systems in electric vehicles and electronic applications (Nasajpour-Esfahani et. al., 2024). In recent years, the need for the development of high-performance Li-ion batteries for use in electric vehicles (EVs) and hybrid electric vehicles (HEVs) has been steadily increasing. (Koech et. al., 2024; Velev et. al., 2024; Çelikbilek et. al., 2022; Lökçü et. al., 2023).

Lithium titanate ($Li_4Ti_5O_{12}$, LTO) has been researched as one of the most suitable anode materials for energy storage systems such as hybrid electric vehicles (HEVs). LTO is an intercalation-type anode material with a spinel structure. Due to its better safety and cycle stability compared to graphite anodes, it holds the second-largest market share in the Li-ion battery industry after graphite (Zhang et al., 2022). The superior properties of

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the LTO anode are mainly due to the phase transformation between $Li_4Ti_5O_{12}$ and $Li_7Ti_5O_{12}$ that occurs during charge/discharge reactions (Ge et al., 2009). These two phases, which belong to the Fd3m space group, have very similar lattice parameters, resulting in a volume change of less than 0.2% during charging/discharging. This gives LTO exceptional cycle stability (Ariyoshi et al., 2005). The working potential of LTO (1.55 V vs. Li^+/Li) is high and prevents dendrite formation. Additionally, this potential is higher than the reduction potentials of most electrolytes and solvents (< 1.0 V), which means a thinner solid electrolyte interphase (SEI) layer forms (He et al., 2012; Zhang et al., 2022). Typically, thick SEI layers consume the active material, leading to capacity loss and low Li^+ diffusion in electrodes (Zhang et al., 2022).

Currently, $LiCoO_2$ is used as the cathode in the majority of commercial Li-ion batteries. However, due to its relatively low capacity (160 mA h g^{-1}) and the limited utilization of lithium within its structure (< 60%), further research into cathode systems has been necessary. In recent years, as electric vehicles have become more common, the main approach to cathode design has been the gradual replacement of cobalt with nickel. This has led to capacities reaching up to 220 mA h g^{-1}, with lithium utilization rates approaching 80%. In these cathode materials, nickel is used for its capacity-enhancing properties, while cobalt and manganese contribute to structural integrity. LiNi-Mn-Co-O_2 cathodes, commonly referred to as NMC, are widely studied materials today (Malik et. al., 2022; Liu et al., 2015). NMC materials have a layered rock salt structure. In this group of cathodes, the chemical composition ranges from $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ (NMC111) to $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811) (Chen et. al., 2024; Murdock et al., 2021; Yu et. al., 2014). Due to its high voltage (3.7–3.9 V), good cycle life, structural stability, safety, and cost-effectiveness, NMC is a suitable cathode material when combined with LTO (Houache et. al., 2022; Farhat et. al., 2017). In this study, the NMC622 ($LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$) cathode electrode and LTO anode electrode were prepared, and the electrochemical performance of Li-ion batteries was investigated.

Materials & Methods

The cathode and anode electrode slurries were prepared using similar parameters. Commercially available NMC622 and LTO active materials were mixed with Super P carbon black and PVDF in NMP medium at specific stoichiometric ratios using a vortex mixer. The prepared anode and cathode slurries were coated onto carbon-coated aluminum foil using a doctor blade, and subsequently dried under vacuum at 80°C for 12 hours. The electrochemical tests of the full cell, composed of an NMC622 cathode and LTO anode, were carried out in a CR2032 coin cell. The assembly of the coin cells was performed in an argon-filled glovebox where H_2O and O_2 levels were kept below 0.1 ppm. As the electrolyte, 1 M Lithium hexafluorophosphate ($LiPF_6$) was used in EC: DMC in a ratio of by 1:1 by volume. Polipropilen (Celgard 2400) membrane was employed as the separator. Charge-discharge tests were conducted using a Gamry Reference 3000 Potentiostat/Galvanostat/ZRA within a potential range of 1.25–2.75 V (vs. Li^+/Li). The assembled cells were first activated at a rate of 0.1 C for 2 cycles within the voltage range of 1.25–2.75 V (vs. Li^+/Li), followed by electrochemical performance testing for 100 cycles at rates of 0.5 C, 1 C, 2 C, and 5 C. X-ray diffraction (XRD) analyses were performed on a PANalytical Empyrean diffractometer with Cu Kα radiation at a scanning rate of 2° min^{-1}.

Results and Discussion

The XRD patterns of the NMC622 electrode on the carbon-coated Al surface are presented in Figure 1. The XRD peaks confirm the layered hexagonal α-$NaFeO_2$-type structure with an R3m space group.The diffraction peaks corresponding to the (003), (101), (006), (102), (104), (105), and (107) planes confirm the crystal structure of NMC. The strong (003) peak observed at $2\theta = 19°$ indicates the well-defined crystalline structure of NMC622 (Loghavi et al., 2022). In addition, a diffraction peak observed around $2\theta = 28°$ is attributed to the presence of carbon in the electrode structure.

The XRD patterns of the LTO electrode coated on the carbon-coated Al surface are presented in Figure 2. The diffraction peaks observed at the (111), (311), (400), (331), and (333) planes indicate a well-defined crystalline structure of the LTO material. In addition to the characteristic peaks of LTO, a peak observed around $2\theta \approx 28°$ is attributed to the presence of carbon in the electrode structure. This carbon peak originates from the conductive carbon additives used in the electrode formulation and/or the carbon coating on the aluminum current collector.

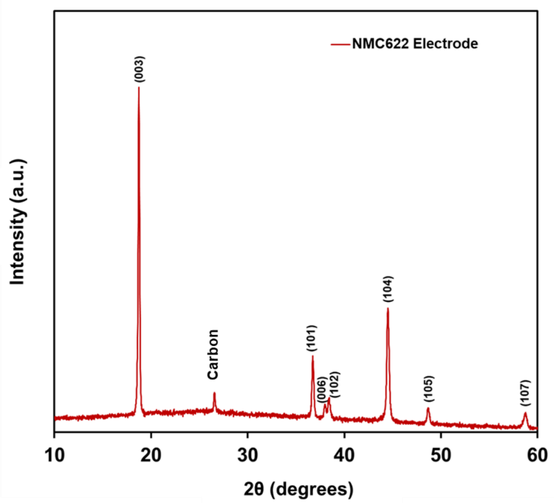

Figure 1. XRD patterns of the NMC622 electrode.

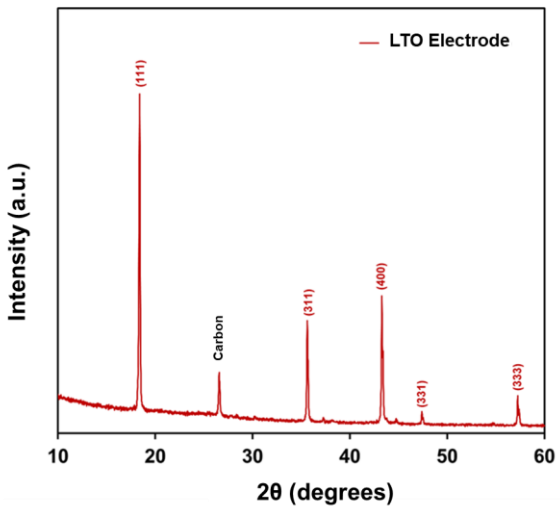

Figure 2. XRD patterns of the LTO electrode.

The charge/discharge test of the full cell composed of an LTO anode and NMC622 cathode, conducted at 0.1 C within the voltage range of 1.25–2.75 V (vs. Li^+/Li) for 2 cycles, is presented in Figure 3. At the end of the second cycle, the charge capacity was determined to be approximately 159 mA h g^{-1}, while the discharge capacity was approximately 145 mA h g^{-1}.

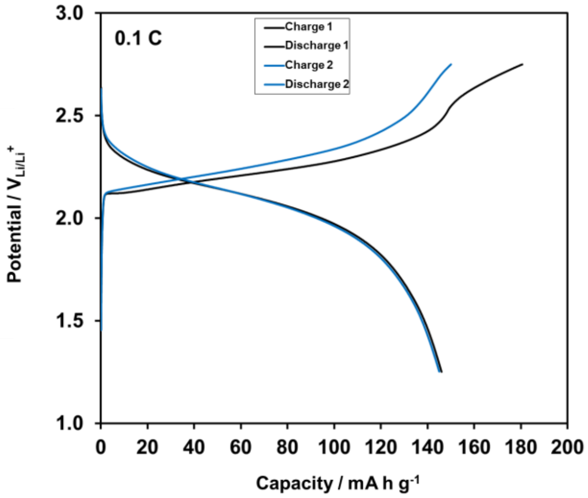

Figure 3. Charge and discharge curves of the LTO anode – NMC622 cathode full cell at a 0.1 C rate.

The effect of different charge/discharge rates on the cycling performance of the full cell comprising an LTO anode and NMC622 cathode was evaluated over 100 cycles at 0.5 C, 1 C, 2 C, and 5 C. The corresponding charge/discharge profiles are shown in Figures 4a–4d. The variation of charge and discharge capacities with cycle number for each C-rate is comparatively presented in Figure 5.

At the initial cycle, the discharge capacities were measured to be 127 mA h g^{-1}, 120 mA h g^{-1}, 105 mA h g^{-1}, and 70 mA h g^{-1} at 0.5 C, 1 C, 2 C, and 5 C, respectively. After 100 cycles, these values decreased to 81 mA h g^{-1}, 68 mA h g^{-1}, 64 mA h g^{-1}, and 50 mA h g^{-1}, indicating a gradual capacity fade with increasing current rates. Across all tested C-rates, the coulombic efficiency remained stable in the range of 90–95%, suggesting good reversibility of the electrochemical reactions. Furthermore, the capacity retention after 100 cycles ranged from 65% to 70%, reflecting moderate long-term stability under varying rate conditions.

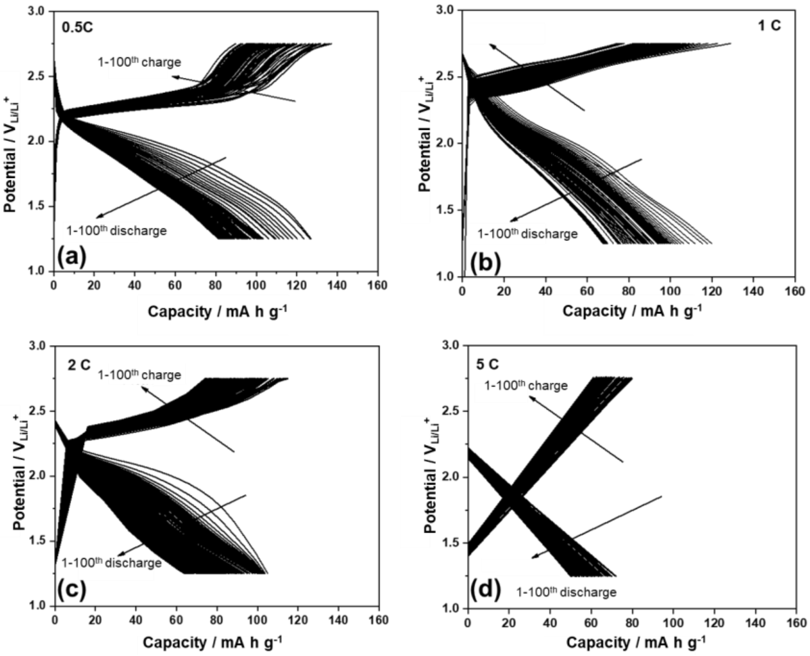

Figure 4. Performance of the full cell with LTO anode – NMC622 cathode in the potential range of 1.25–2.75 V (vs. Li$^+$/Li) at (a) 0.5 C, (b) 1 C, (c) 2 C, and (d) 5 C rates over 100 cycles.

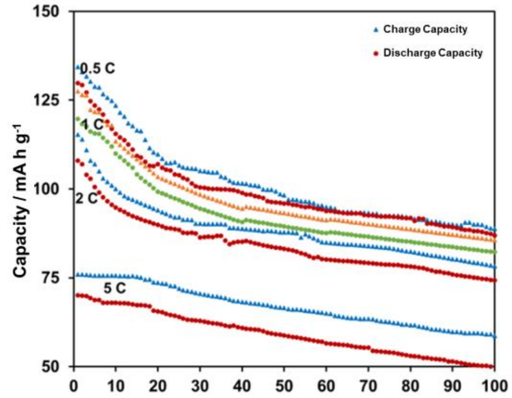

Figure 5. Comparison of the charge and discharge capacities of the full cell with LTO anode – NMC622 cathode at 0.5 C, 1 C, 2 C, and 5 C rates over 100 cycles.

Conclusion

In this study, electrodes were prepared using LTO as the anode and NMC622 as the cathode material. The crystal structures of the anode and cathode electrodes were characterized using X-ray diffraction (XRD) technique. The electrochemical performance of the lithium-ion batteries was evaluated. Charge-discharge measurements showed that the full cell exhibited a discharge capacity of 50 mAh g^{-1} after 100 cycles at a 5 C rate, with a capacity retention of 70%.

In conclusion, the full cell combining LTO anode and NMC622 cathode materials demonstrates acceptable capacity and cycling stability even at high C rates, making it a promising candidate for practical lithium-ion battery technologies. The results support the applicability of such material systems in applications requiring rapid energy delivery and indicate potential for further improvement through future optimization studies.

Scientific Ethics Declaration

* The authors declare that the scientific ethical and legal responsibility of this article published in EPSTEM journal belongs to the authors.

Conflict of Interest

* The authors declare that they have no conflicts of interest

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