Data Article

Dataset on a primary lithium battery cell with a ferroelectric Li-glass electrolyte and MnO₂ cathode

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Abstract

Here we show the electrochemical data for a Ferroelectric Electrolyte Battery (FEB) Li/ferroelectric Li-glass electrolyte (Li2.99Ba0.005ClO) in cellulose/γ-MnO₂ pouch-cell with (2.5 × 2.5 cm²) discharged with a green LED load. The Li2.99Ba0.005ClO electrolyte was synthesized and ground in ethanol. A cellulose matrix was dipped into the Li-glass/ethanol slurry. The γ-MnO₂ based cathode was doctor bladed onto a carbon-coated aluminum foil current collector. The cell was assembled in an Ar-filled glove-box and it was not sealed and, therefore, it remained inside the glove-box while discharging with a green LED at approximately 24 °C for 334 days (>11 months) corresponding to 764 mAh g⁻¹ of the active cathode and to 224 mAh g⁻¹ of the electrolyte. The maximum capacity of γ-MnO₂ is 209 mAh g⁻¹ and of the MnO₂ in the commercial cell is 308 mAh g⁻¹, corresponding to LiMnO₂; therefore, the capacity of the FEB is 370% the capacity of the γ-MnO₂ and 250% the capacity of the MnO₂ in the commercial cell. Moreover, the experimental capacity of the electrolyte minus the maximum capacity of the γ-MnO₂ is 163 mAh g⁻¹ of the electrolyte. The potential difference between anode and cathode in a diode is non-linear and dependent on the input current and, therefore, the plateaus in the potential vs time curves do not correspond to thermodynamic equilibria of the electrochemical cell energy source. Nevertheless,

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the maximum output current as well as the FEB cell’s discharge profile may be determined with an LED and compared with traditional battery cells' profiles. The present data might be used by the electrochemical (in particular, battery), electrostatic and ferroelectric materials researchers and industrials for comparative analysis. Furthermore, it can be reused to calculate the maximum energy stored electrostatically in these devices.

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| Specifications Table |
|----------------------|
| Subject | Materials Science (General) |
| Specific subject area | Electrochemical and electrostatic characterization of a solid-state primary battery. |
| Type of data | Performance of a ferroelectric electrolyte |
| How data were acquired | Chart |
| Data format | Table |
| Parameters for data collection | Photograph |
| Description of data collection | How data were acquired | Electrochemical discharge |
| | Instrument: Bio-Logic VMP300 potentiostat |
| | Photographs |
| | Instrument: cell phone |
| Parameters for data collection | A FEB Li/ferroelectric Li-glass electrolyte/g-MnO2 pouch-cell, m(g-MnO2) = 16.24 mg was discharged while lighting a green LED during 334 days. The cell was not fully discharged. The potential vs time, V vs t, its corresponding current vs time, I vs t, and capacity vs time, Q vs t, discharge curve were obtained. I vs t, was determined after obtaining the discharge profile V vs I of the LED. A commercial CR1616 cell Li/Liquid electrolyte/MnO2 mminimum(MnO2) = 216 mg corresponding to LiMnO2 was discharged in the same conditions serving as a control experiment. |
| Parameters for data collection | Description of data collection | The V vs t data was collected by associating a green LED, the FEB and a potentiostat in parallel. The potentiostat is a BioLogic VMP300. The data was collected each 10 s during 334 days corresponding to 2.895 × 10^6 points. I vs t and Q vs t are also presented and each correspond to the same number of data points as V vs t. |
| Parameters for data collection | Description of data collection | A profile of the green LED, V vs I, function was determined with the same potentiostat as well as the V vs t, I vs t, and Q vs t data for a commercial cell which were also collected each 10 s corresponding to 6.142 × 10^4 data points in each curve. The green LED and the CR1616 Li–MnO2 coin-cell are wide access commercial products. |
| Data source location | Data source location | Institution: UPORTO |
| | City/Region: Porto |
| | Country: Portugal |
| Data accessibility | Repository name: Mendeley |
| | Data identification number: Mendeley Data |
| | Direct URL to data: https://doi.org/10.17632/rydhr7j4vj.1 |
| Related research article | Related research article | Authors: M. H. Braga, A. J. Murchison, J. E. Oliveira, J. B. Goodenough |
| | Title: Low-Temperature Performance of a Ferroelectric Glass Electrolyte Rechargeable Cell |
| | Journal: ACS Appl. Energy Mater. 2(7) (2019) 4943–4953 |
| | doi: 10.1021/acsaeem.9b00616 |

**Value of the Data**

- The data presents the electrochemical discharge behavior of a cell that shows a capacity which is 370% the theoretical capacity of active cathode (g-MnO2) while not fully discharged, conversely to traditional batteries which seldom surpass 80% of the cathode’s theoretical capacity; It is therefore of practical and theoretical interest to make these data accessible to facilitate comparisons.
- The scientific and industrial community can benefit from these data while studying disruptive solid-state devices that are neither traditional batteries nor capacitors.
- These data can be used to develop experiments with other ferroelectric all-solid-state electrolyte energy storage cells.
- These data show comparison between a ferroelectric electrolyte battery (FEB) and a commercial cell with very different discharge profiles and capacities; it is, therefore, possible to study the electrostatic process that occurs beyond the electrochemical process.
1. Data description

All the data plotted in Fig. 1 may be obtained from the files accessible in the database:

![Image](image-url)

**Fig. 1.** Discharging performance of a Li/ferroelectric Li-glass electrolyte/γ-MnO₂ FEB pouch-cell with \( m(\gamma\text{-MnO}_2) = 16.24 \text{ mg} \) while lighting a green LED in an Ar filled glove-box. Comparison with the performance of a Li/Liquid electrolyte/γ-MnO₂ commercial CR1616 coin-cell with an active cathode \( m(\text{MnO}_2) = 216 \text{ mg} \). The mass of the active cathode surface in contact with the electrolyte in the CR1616 is at least 1330% the mass of the active cathode surface of the FEB pouch-cell as, while the FEB is 1D contact, the CR1616 is a 3D contact since the liquid electrolyte, conversely to the solid, wets all the cathode. Variable potential and current.

- **a)** Potential vs time for the FEB and CR1616;
- **b)** Current vs time for the FEB and CR1616;
- **c)** Potential vs specific capacity for the FEB and CR1616;
- **d)** Photograph of the green LED connected to a FEB pouch-cell;
- **e)** Photograph of the green LED (not shown) after discharging for 334 days;
- **f)** Potential vs specific capacity for the FEB pouch cell, as a function of the active cathode \( (\gamma\text{-MnO}_2) \), as traditionally calculated, since the cathode usually shows the lowest capacity defining the cell’s capacity; as a function of the electrolyte’s mass **g)** which, in a traditional cell, does not contribute to the capacity of the cell.
(1) V_vs_time_1.txt (compressed in a zip file) (Fig. 1a);

Discharging performance of a Li/ferroelectric Li-glass electrolyte/\(\gamma\)-MnO\(_2\) FEB pouch-cell with \(m(\gamma\text{-MnO}_2) = 16.24\) mg and \(m(\text{Li-glass}) = 55.3\) mg while lighting a green LED inside an Ar-filled glove-box. The file contains two columns (time/s, potential/V); the data were obtained each 10 s during 334 days corresponding to \(2.895 \times 10^6\) data points.

(2) I_vs_time_1.txt (compressed in a zip file) (Fig. 1b);

The file contains two columns (time/s, current/\(\mu\)A) correspondent to the discharge of the cell in Refs. [1] for 334 days with \(2.895 \times 10^6\) data points; the data were obtained using [1] and the green LED’s V vs I discharge profile.

(3) Q_vs_time_1.txt (compressed in a zip file);

The file contains two columns (time/s, capacity/mAh); the data were obtained integrating (2) for 334 days corresponding to \(2.895 \times 10^6\) data points.

(4) V_vs_time_comercial_4.txt (compressed in a zip file) (Fig. 1a);

Discharging performance of a Li/liquid electrolyte/MnO\(_2\) commercial CR1616 coin-cell with a minimum active material \(m(\text{MnO}_2) = 216\) mg (for 100% efficiency) while under a green LED load. The file contains two columns (time/s, potential/V); the data were obtained each 10 s during 7.1 days corresponding to \(6.143 \times 10^4\) data points. The cell could not be observed lit after 6 days and 14 hours.

(5) I_vs_time_comercial_5.txt (compressed in a zip file) (Fig. 1b);

The file contains two columns (time/s, current/\(\mu\)A) from the discharge of the cell in (4); the data were obtained during 7.1 days, corresponding to \(6.143 \times 10^4\) data points, using (4) and the green LED V vs I profile.

(6) Q_vs_time_comercial_6.txt (compressed in a zip file);

The file contains two columns (time/s, capacity/mAh); the data were obtained integrating (5) for 7.1 days corresponding to \(6.143 \times 10^4\) data points.

Remarks for (1) to (3): while the pouch cell was in the glove box for 334 days under the green LED load, a glitch happened due to a touch in the potentiostat’s cables that resulted in a quick loss of contact. It happen after 4.9 days and it was immediately solved; the correspondent potential data were removed although the time was counted since the cell kept on being discharged.

General remarks (1) to (6): the first rows identify the cell and its parameters.

(7) pouch-cell_green_LED.pdf

Photographs of the green LED while connected in parallel to the FEB pouch-cell and potentiostat (both not shown) for days: 1, 11, 12, 17, 34, 40, 42, 43, 46, 51, 56, 64, 70, 77, 82, 89, 96, 117, 138, 154, 186, 197, 215, 225, 232, 258, 307, 326, and 334 (Fig. 1e).

2. Experimental design, materials, and methods

Five grams of a Li\(^+\) ferroelectric glass electrolyte was synthesized by adding approximately 20 ml of deionized water to \(2.3317\) g of LiCl, \(2.6212\) g of Li(OH), and \(0.0471\) g of Ba(OH\(_2\)) precursors of Li\(_{2.98}\)Ba\(_{0.005}\)ClO (LiOH - Sigma Aldrich 98% pure, LiCl - Sigma Aldrich ≥99% pure, Ba(OH\(_2\)) – Sigma
Aldrich ≥ 95% pure). The reagents were added, mixed, and closed in a Teflon reactor, which was partially immersed in a sand bath that was heated to 80 °C. After around 2 hrs, it was verified that the reagents were all well-dissolved. The bath was then slowly heated to 230–240 °C and left at this temperature until all the water evaporated. The water evaporated from a loose cap that was slightly unscrewed after having cooled down the Teflon reactor to a safe temperature (<80 °C) and subsequently heated it to 230–240 °C again. Verification that the water has evaporated is made by cooling the reactor one more time until it can be safely opened; a white solid is deposited on the Teflon reactor if the water is all dried out. The reactor with the electrolyte content is then placed in an argon-filled glove box (H2O < 0.1 ppm and O2 < 1 ppm). The cell was fabricated and tested in a MBraun argon-filled glove-box. The FEB Li/Li+–glass/γ-MnO2 pouch-cell was assembled after making an absolute ethanol Li+-glass ferroelectric electrolyte slurry in which a cellulose squared membrane with >2.5 × 2.5 cm² was embedded and left to dry inside the glove-box. An asymmetric cell containing γ-MnO2 as active material (m = 16.4 mg) coated on the surface of a carbon coated Al current collector with a lithium negative electrode and the Li-glass cellulose composite membrane, separating both electrodes, was assembled with an active square surface area of approximately 2.5 × 2.5 cm² (Fig. 1d). The cathode loading for the asymmetric cell was determined to be 81.6% active material, 6.4% acetylene black, 4% Timcal Super P graphite, and 8% PVDF; both slurries were doctor bladed onto a carbon-coated Al foil current collector. The cathode film was vacuum dried at 80 °C for 12 hours. The amount of electrolyte embedded in the cellulose matrix of the coin-cells was 55.3 mg.

The pouch cell was never sealed; it remained in the glove box during assembly and the 334 days of electrochemical testing (Fig. 1d). A primary commercial Li–MnO2 CR1616 coin-cell with capacity of approximately 66 mAh (cut off 2V), theoretical capacity of 308 mAh/g (LiMnO2) corresponding to a minimum amount of active cathode of 216 mg (for an 100% efficiency) was also tested as a reference of the discharge method. The wide available commercial green LED was profiled to obtain a detailed potential vs current correspondence for all the potential range tested. The instrument used was a Bio-Logic VMP300 potentiostat. The potentiostat’s original cable connects to the LED inside the Ar-filled glove-box which is connected to the FEB pouch-cell which was assembled and tested in the glove box.

Photographs were taken with cell phones through the glove-box glass window.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2020.105339.

References

[1] M.H. Braga, A.J. Murchison, J.E. Oliveira, J.B. Goodenough, Low-temperature performance of a ferroelectric glass electrolyte rechargeable cell, ACS Appl. Energy Mater. 2 (7) (2019) 4943—4953.