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Cell Performance of Ultra-Thin Polymer Cathode System:
Theoretical Energy and Power Density Projections

by

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Theoretical energy and power density values for thin film Li/liquid/electrolyte/ polymer cell systems were calculated by designing a specific cell model for both a prismatic cell with only the basic cell elements (no hardware) and a bipolar-design cell with some idealized practical hardware. The cell performance is compared for three different cathode polymer materials, viz., polyaniline, polypyrrole, and polyvinylferrocene. The energy and power densities are estimated as a function of cathode thickness, active cell area, and initial concentration of electrolyte for very thin cathode films (cathode thickness: $L_c^l = 1$ to $100\mu m$) in both single cell and bipolar designs. The energy and the power estimated at 80 Wh/kg and 800 kW/kg for $10\mu m$ cathodes. Problems of battery manufacturing process were not addressed.

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Conducting polymers as well as polymeric redox materials are regarded to have high electroactivity in organic liquid electrolytes. These materials can be utilized as one of the promising candidates for cathode materials in future rechargeable cell systems. Polymer cathode cells, in general, are known to have a lower energy density when compared to inorganic intercalation materials such as the oxides or sulfides of Ti, Mo and V. However, this type of conducting polymer material exhibits very fast kinetics in exchanging electrons as well as ions during the charge/discharge process. The rapid kinetics should lead to high power densities. So, this type of polymer material is considered to be high power material rather than high energy material. The present paper reports theoretical calculations of specific energy and specific power for secondary lithium cells using three different polymer cathode materials, viz., polyaniline, polypyrrole and polyvinylferrocene. The particular emphasis of this paper is to indicate how much energy or power one may obtain from these polymer materials and the optimum conditions for certain of the fundamental cell design parameters including thickness and area.

Unit Cell with Basic Cell Elements

The theoretical energy and power density calculations are relatively straightforward for a prismatic cell without hardware or separator. The table below summarizes the values of ED and PD_{max} for three different Li/polymer cathode cell systems, where the thickness of each cathode is fixed at 1, 10 and 100μm. Balanced electrodes were assumed.

The maximum power density is obtained at the half value of voltage($E_{oc}/2$) and current(I/2) in the load curve where only the electrolyte polarization is taken into account[1].

$$PD_{max} = \frac{E_{oc}^2}{4} \cdot \frac{S}{\rho L_e} \cdot \frac{1}{W_{cell}}$$, where ρ is the resistivity of the electrolyte. Le is the electrolyte thickness, and S is the area of the electrode. If one considers a cell with a capacity of 1 Faraday (96500) coulombs, or 26.8 Ah), the W_{cell} for a Li/4M LiClO₄(PC)/Polymer cell can be derived from cathode weight.

### Cell Performance of Li/4M LiClO₄(PC)/Polymer Cells (No Hardware)

	PAn	PPy	PVF
E_{oc} [V] (0% DOD)	4.0	3.5	3.85
E_{oc} [V]	3.7	3.0	3.5
Specific Gravity [g/cm³]	1.08	1.48	0.42
Maximum Doping Level [%]	80	40	100
Molecular Weight(1 unit) [g/mol]	91	65	212
Energy Density [Wh/kg]	152	140	128
Energy Density [Wh/liter]	290	255	140
Specific Power [W/kg] Le = 1 μm	160 M	120 M	2.9G
Specific Power [W/kg] Le = 10 μm	16 M	1.2 M	29 M
Specific Power [W/kg] Le = 100 μm	16 K	12 K	290 K

Bipolar-design Battery(Li/4M LiClO₄(PC)/Polyaniline)

A practical cell configuration would consist of the cell plus some basic hardware. The energy and power densities for bipolar-design cell which consists of (X+1) cells in series were calculated. There are X bipolar cells plus the terminal electrodes; this type of cell reduces to a single prismatic cell design when the number of bipolar units are equal to 0. The following assumptions were made for this battery design; (1) f_{ex} (excess factor)= 3, i.e., Q_{Li} = $3Q_{cathode}$, (2) terminal Ni electrode 25 μm (1mm wider than R_{cell}), (3) Current collector in bipolar unit(Al) thickness=20% of L_{cell} (1mm wider than R_{cell}), (4) Case(Synthetic resin) $R_{case} = R_{cell} + 2$ mm, where R_{cell} is the radius of the circular cell.

Surface Area = S
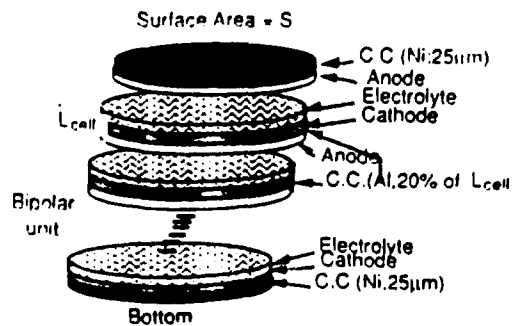
The above figure shows the battery construction of the bipolar electrode cells which were used for the energy and power calculations of the Li/Polymer cathode cell system. Separators were ignored for these conclusions. Two kinds of hardware are included in this type of cell, namely, the current collectors and the case wall. The current collector involves the plates of Ni and the Al bipolar inter cell connector. The Ni current collector is much harder and more dense than the Al current collector, and is suited for the terminal electrode. On the other hand, the Al current collector is more flexible and lighter, and the thickness was assumed to be 20% of the active cell thickness(L_{cell}), unless the $L_{cell} > 150$ μm. Then the thickness of Al was fixed at 30 μm. For the wall material, the authors assumed a synthetic resin(d=0.8 g/cm³), that encapsulated the entire cylindrical battery. For the electrolyte solution, 4 M LiClO₄(PC)(σ=3.0×10⁻³ S cm⁻¹) was assumed in the fully discharged state of the cathode.
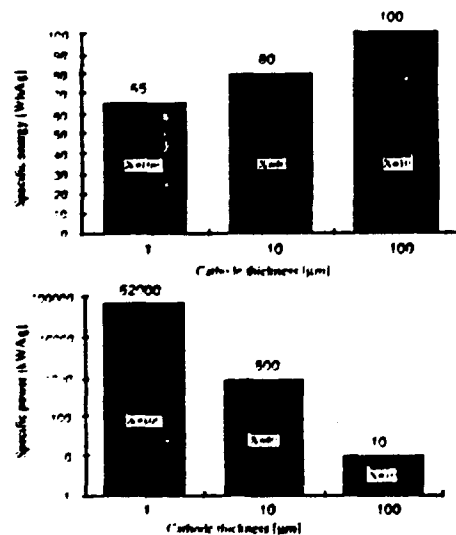
The above figure shows the best values for specific energy and power for the bipolar-design battery. The ED and PD values exhibit maxima at reverse directions in terms of cathode thickness.

References

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