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Computer simulations of the influence of geometry in the performance of conventional and unconventional lithium-ion batteries

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HIGHLIGHTS

- The influence of geometries in lithium-ion battery performance is analyzed.
- Conventional and unconventional battery geometries are investigated.
- Unconventional geometries include horseshoe, spiral, ring, antenna and gear batteries.
- The best capacity value at 330 C is obtained for the interdigitated geometry.
- The capacity value is dependent on thickness and collectors position.

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ABSTRACT

In order to optimize battery performance, different geometries have been evaluated taking into account their suitability for different applications. These different geometries include conventional, interdigitated batteries and unconventional geometries such as horseshoe, spiral, ring, antenna and gear batteries. The geometry optimization was performed by the finite element method, applying the Doyle/Fuller/Newman model. At 330 C, the capacity values for conventional, ring, spiral, horseshoe, gear and interdigitated geometries are 0.58 A h m^{-2}, 149 A h m^{-2}, 182 A h m^{-2}, 216 A h m^{-2}, 289 A h m^{-2} and 318 A h m^{-2}, respectively.

The delivered capacity depends on geometrical parameters such as maximum distance for the ions to move to the current collector, *d*_max, distance between of current collectors, *d*_cc, as well as the thickness of separator and electrodes, allowing to tailor battery performance and geometry for specific applications.

1. Introduction

Energy storage systems are an essential need in a modern society with rapid technological advances, increasing mobility and environmental concerns [1–3], the most used energy storage systems being lithium-ion batteries [4,5].

Lithium-ion batteries are essential in applications such as mobile-phones and computers, among others. Further, they area also explored for hybrid electric vehicles (PHEVs) and electric vehicles (EVs) [6–8].

Lithium-ion batteries dominate the battery market with a share of 75% due to their advantages with respect to other battery systems (NiCd, nickel-cadmium and NiMH, nickel-metal hydride), including high energy density, lightweight, high average discharge rate, no memory effect and high cycle life [9,10].

The key issues for lithium-ion batteries are related to improving specific energy, power, safety and reliability [5]. These issues strongly depend on the materials for electrodes (anode and cathode) and separator (porous membrane with electrolyte solution) [11–14].

Together with the materials, also the geometry of the battery strongly affects its performance, the interdigitated geometry being the most investigated for this effect [15–17].

The interdigitated geometry is based on electrode digits separated by an electrolyte, allowing increased surface area for the

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Nomenclature

List of symbols

a	specific interfacial area, m^2/m^3
C_L	concentration of Li ions in the electrolyte, mol/m^3
$C_{E,i}$	concentration of Li ions in the electrode i ($i = a, c$), mol/m^3
D_l	diffusion coefficient of the salt in the electrolyte, m^2/s
$D_{ef,i}$	effective diffusion coefficient of the salt in the electrolyte i ($i = a, s, c$), m^2/s
D_{LI}	diffusion coefficient of Li ions in the electrode, m^2/s
F	Faraday's constant, 96,487 C/mol
$f_{\pm}$	activity of the salt in the electrolyte, mol/m^3
$\mathbf{i}_E$	current density in the electrode, A/m^2
$\mathbf{i}_L$	current density in the electrolyte phase, A/m^2
I_{TOTAL}	total current density, A/m^2
j^{+}_{Li}	pore wall flux of Li ions, $mol/cm^2\,s$
L_i	electrode thickness i ($i = a, c$), m
c_dig	digit length of the electrode, m
e_dig	digit thickness of the electrode, m
e_sep	separator thickness, m
d_max	maximum distance of ions more distant of collectors positions
d_cc	distance between of collectors
R_d	radius of ring geometry, m
R_g	radius of gear geometry, m
L_dim	dimension of horseshoe, m
$\mathbf{M}$	mass transport flux, mol/m^2
$\mathbf{R}$	reaction term of the mass balance equation, $mol/m^3\,s$
R	gas constant, 8314 J/mol K
R_f	film resistance, $\Omega\,m^2$
r	radius of the electrode spherical particles, m
T	temperature, K
t	time, s
t^0_+	transport number of the positive ions
u^0	open circuit voltage, V
N	number of digits for interdigitated and gear battery
A_i	area of a given component in the battery i($i = a, s, c$)
p	porosity of the separator
brugg	brugg parameter of the electrodes

Greek symbols

ε_i	porosity of region i ($i = a, s, c$)
$\varepsilon_{f,i}$	volume fraction of the fillers in the electrode i ($i = a, s, c$)
τ	tortuosity of the separator
η	over-potential, V
φ_E	potential of the electrodes, V
φ_L	potential of the electrolyte, V
κ_l	ionic conductivity of the electrolyte, S/m
$\kappa_{ef,i}$	effective ionic conductivity of the electrolyte i ($i = a, c$), S/m
κ_f	effective ionic conductivity of the separator polymer film, S/m
σ	electronic conductivity of the solid phase of the electrode i ($i = a, s, c$), S/m
$\sigma_{ef,i}$	effective electronic conductivity of the solid phase of the electrode i ($i = a, s, c$), S/m

Subscripts referring specific components of the battery and initial condition

a	anode
c	cathode
s	separator
0	initial condition

electrodes. In this geometry, the Li^+ transport paths are shorter, reducing the electrical resistances across the battery and ion diffusion [16,18].

As an example, lithium-ion microbatteries with interdigitated electrodes have been fabricated by electrodepositing high capacity electrolytic materials, manganese oxide cathode and lithium anode. The capacity value of these microbatteries is 29.5 μA h/cm² μm, with an increase in capacity and power by 10× and 1000×, respectively, in comparison with conventional batteries [16,19].

Microbatteries based on interdigitated geometries have been fabricated by printing $Li4Ti_5O_{12}$ (LTO) and $LiFePO_4$ (LFP) based inks. These batteries show high energy density, 9.7 J cm^{-2}, at a power density of 2.7 mW cm^{-2} and can be used in microelectronics and biomedical devices [20].

The combination of printing technologies and microbatteries allow to obtain customizable thin batteries with large area and at low-cost [21]. These batteries can be fabricated with specific geometries by different printing (screen, spray and inkjet printing) techniques, depending on the final applications. Thus, it has been demonstrated that it is possible to fabricate microbatteries by ink-jet printed that operate at 90 C [22].

Printed battery applications include radio-frequency identification (RFID), security, thin film medical products and products that require on-board battery power [23]. Thus, evaluation of the possible battery geometries is necessary for optimizing size, fabrication and integration before experimental implementation. The optimization of the geometries can be carried out through computer simulations of battery performance [24].

Battery performance by computer simulation is based in models at different physical levels describing the physical–chemical properties of the materials to be used as electrodes and separators, as well as the operation of the battery [25–27].

These computer simulations are thus essential for battery development as they allow the correlation between theoretical and experimental results through the electrochemical behavior of the batteries [28].

The state-of-the art regarding battery geometry optimization of lithium-ion batteries through simulation models include interdigitated [16,18,29,30], cylindrical [31,32], spiral wound [33] and prismatic geometries [34]. For these geometries, thermal analysis has been performed [32,34–36]. Further, different active material shapes for the for anode, i.e., different microstructures, [37] have been evaluated as well as the effect of thickness [38]. Further, the effect of lithium distribution and concentration [39] and geometric characteristics, i.e., porosity and tortuosity [40] have been computer simulated. Finally, a theoretical analysis of potential and current distributions has been carried out for lithium-ion batteries with planar electrodes [41].

The most relevant geometry for increasing capacity value is the interdigitated geometry [19].

Taking into account the advantages of printing techniques allowing battery fabrication with unconventional geometries, which will improve device integration and overall performance for different application, the novelty of this work is to quantitatively evaluate the effects of seven different lithium-ion battery geometries while maintaining constant the area of the different components. In this way, just the effect of geometry variation is quantified. Five of the evaluated geometries have never been reported before. Battery performance has been determined up to 500 C, as microbatteries fabricated by printing batteries are