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Citation: AIP Conference Proceedings **1738**, 370010 (2016); doi: 10.1063/1.4952155
View online: http://dx.doi.org/10.1063/1.4952155
View Table of Contents: http://scitation.aip.org/content/aip/proceeding/aipcp/1738?ver=pdfcov
Published by the AIP Publishing

Evaluation and Optimization of the Performance of Frame Geometries for Lithium-Ion Battery Application by Computer Simulation

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Abstract. Tailoring battery geometries is essential for many applications, as geometry influences the delivered capacity value. Two geometries, frame and conventional, have been studied and, for a given scan rate of 330C, the square frame shows a capacity value of 305,52 Ahm^{-2}, which is 527 times higher than the one for the conventional geometry for a constant the area of all components.

Keywords: Simulation, capacity, lithium ion battery.
PACS: 88.80.F-, 88.80.ff, 88.05.-b

INTRODUCTION

Current society, with constant mobility and rapid technological advances, lead to an increasing need of batteries with large autonomy for applications such as mobile-phones, computers, e-labels, e-packaging and disposable medical testers, among others, as well as for hybrid electric vehicles (PHEVs) or electric vehicles (EVs). [1].

Typically, in order to increase the performance of a battery (power and energy density), new materials for electrodes (cathode and anode) and separators are developed and new geometries are explored. It has been shown that an interdigitated geometry is a possible way for developing with high-power and high-energy density batteries [2].

Taking into account that computer simulations of battery performance based on theoretical models at different scales [3] are critical for optimizing geometries before experimental battery fabrication [4-5], in this work, a finite element method simulation has been carried out in order to quantitatively evaluate the performance of a frame geometry for lithium-ion batteries at different scan rates. The optimization of the frame structure was carried out taking into account the length of the side maintaining a constant area for the different components.

The performance of two batteries with different geometries has been evaluated: a conventional geometry and a frame geometry (Figure 1). These geometries are illustrated in Figure 1 (a) for a conventional geometry and in Figure 1 (b) and (c) for two frame geometries: square frame and rectangular frame geometries, respectively.

All simulations are based on the Finite Elements Method and by applying the Doyle/Fuller/Newman model [6]. The equations of this model describe the physical and electrochemical phenomena that occur along the operation of batteries in two dimensions [6]. In order to perform a comparative evaluation of the performance of the batteries with different geometries, the same area was maintained for the different components of the batteries (electrodes, separator and current collectors). Further, the variables ***dc*** and ***dm*** are defined, respectively, by the distance between collectors and the maximum distance of lithium ions in relation to the collectors position, as illustrated in Figure 1.

International Conference of Numerical Analysis and Applied Mathematics 2015 (ICNAAM 2015)
AIP Conf. Proc. 1738, 370010-1–370010-4; doi: 10.1063/1.4952155
Published by AIP Publishing. 978-0-7354-1392-4/$30.00

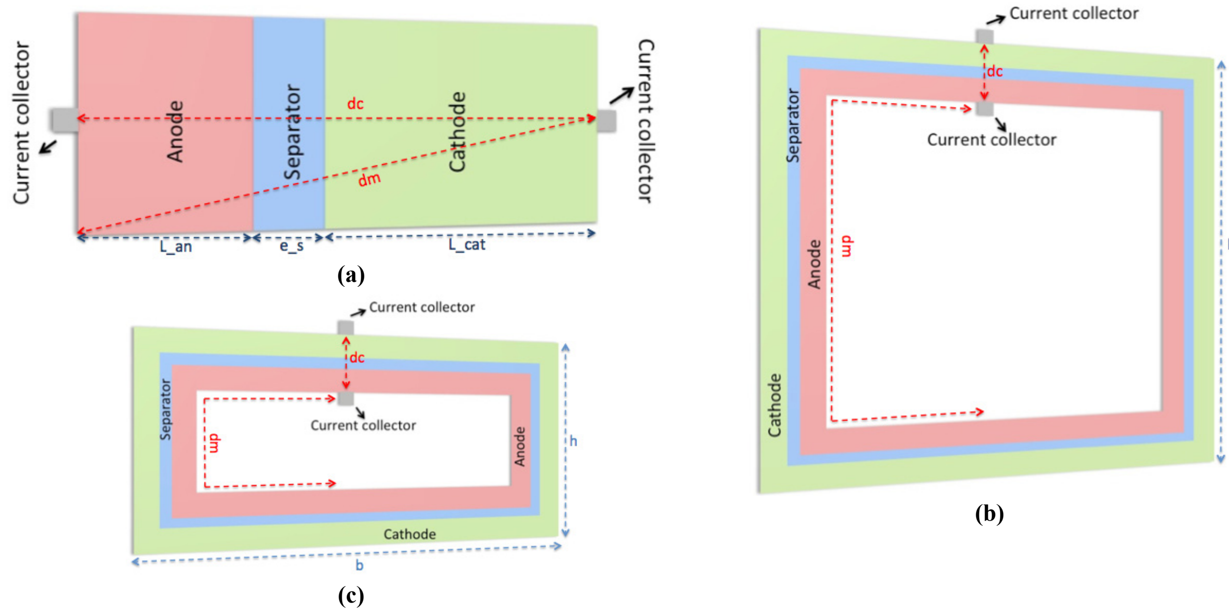


FIGURE 1. Geometries implemented in the simulations and corresponding geometrical parameters (maximum distance, ***dm*** and distance between collectors, ***dc***): (a) conventional geometry, (b) square frame geometry and (c) rectangular frame geometry.

The first part of the study is focused in the evaluation of the capacity value at low, medium and high discharge rates (from 1C up to 500C). For the conventional geometry, the thickness of the anode (***L_an***) was fixed at 200 µm, the thickness of the cathode (***L_cat***) at 400 µm and the thickness of the separator (***e_s***) at 90 µm. In the square frame, it was used a value for the length (***L***) of 100 µm. The influence of the side length for the square frame on the performance of the battery was evaluated at higher discharges rates (500C). The optimal value of the side length of the frame geometry was obtained by adjusting the obtained capacity values as a function of length by a Quadratic Regression Polynomial using the Least Square Method. For the determination of the optimal length value (***L***), it was used the area (***A***) for each component (electrodes and separator) shown in Table 1. Finally, it was determined the capacity value of the square frame and rectangular frame geometries with a given maximum distance (***dm***), equal distance between collectors (***dc***) and the same area of all components in both geometries at 500C of discharge rate. The side length (***L***) for the square frame is 200 µm and the base (***b***) and height (***h***) of the rectangular frame geometry are 300 µm and 100 µm, respectively.

Table 1 shows the parameters used in the battery models for the different geometries.

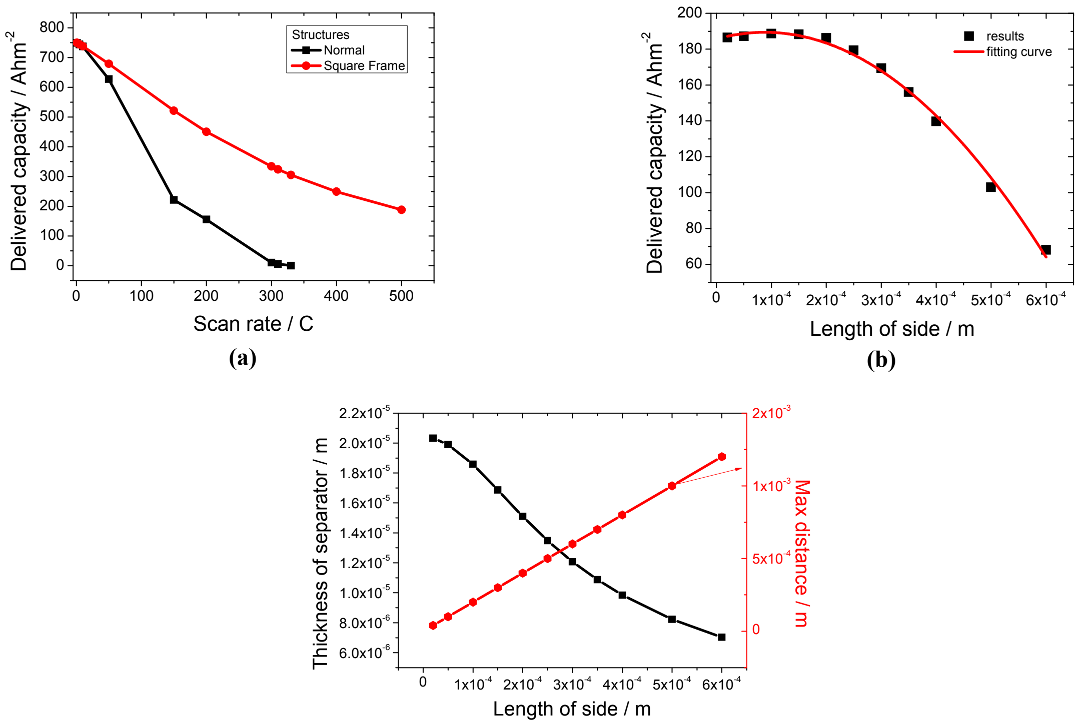
TABLE 1. Parameters used in the simulations of the batteries with different geometries: conventional, square and rectangular frame

Parameter	Unit	Anode (Li_xC_6)	Separator	Cathode ($Li_xMn_2O_4$)
$C_{E,i,0}$	mol/m^3	14870		3900
$C_{E,i,max}$	mol/m^3	26390		22860
C_L	mol/m^3		1000	
r	m	$12{,}5\times10^{-6}$		8×10^{-6}
L_i	m	200×10^{-6}	90×10^{-6}	400×10^{-6}
k_i	S/m	$(6{,}5\times10^{-1})\times0{,}357^{1,5}$	$(6{,}5\times10^{-1})\times4{,}84\times10^{-2}$	$(6{,}5\times10^{-1})\times0{,}444^{1,5}$
D_i	m^2/s	$(4{,}0\times10^{-10})\times0{,}357^{1,5}$	$(4{,}0\times10^{-10})\times4{,}84\times10^{-2}$	$(4{,}0\times10^{-10})\times0{,}444^{1,5}$
D_{LI}	m^2/s	$3{,}9\times10^{-14}$		1×10^{-13}
Brugg or p		1,5	8,5	1,5
$\varepsilon_{f,i}$		0,172		0,259
ε_i		0,357	0,70	0,444
τ			3,8	
σ_i	S/m	100		3,8
i_{1C}	A/m^2		17,5	
T	K		298,15	
A_i	m^2	$4{,}0\times10^{-8}$	$1{,}8\times10^{-9}$	$8{,}0\times10^{-8}$

The choice of the frame geometry is due to the availability of empty space at the center of the battery, as shown in Figure 1 (a). This empty space allows applicability in various portable technologies. Thus, it is important to compare the performance of this geometry with the conventional geometry that is commonly used in commercial batteries.

RESULTS AND DISCUSSION

The Figure 3 (a) shows the capacity values obtained at different discharges rates for the conventional and square frame geometries. The results (Figure 3 (a)) show that the square frame geometry presents a higher performance in comparison with the conventional geometry at different discharge rates. For the conventional geometry, the capacity value is 0,58 Ahm^{-2} for 330C. For the same scan rate, the square frame shows a capacity value of 306,00 Ahm^{-2} (527 times higher than the conventional geometry). It is also observed that the conventional geometry does not work for discharge rates above 330C but, on the other hand, the square frame geometry can operate at higher discharges rates up to 500C. At higher discharge rates it is required a higher ionic flow between electrodes and high ion insertion capacity in the cathode. The square frame geometry contains these requirements as this geometry shows a thin separator and a higher surface contact area between the electrodes.



(c)

FIGURE 2. (a) Delivered capacity as a function of scan rate for conventional and square frame geometries. (b) Delivered capacity as a function of side length of the square frame geometry at 500C. Fitting of the capacity values as a function of side length through a Quadratic Regression Polynomial using Least Square Method. (c) Thickness of the separator and maximum distance as a function of the side length of the square frame geometry.

Figure 2 (b) shows the influence of side length of the square frame in the capacity value at 500C. The length of the side was changed from 20 μm to 600 μm. In the length range from 20 μm to 100 μm it is observed an increasing capacity value, but in the range of lengths from 100 μm to 600 μm it is verified a decrease in the capacity value. For 20 μm of side length the capacity value is 187,01 Ahm^{-2} and 188,72 Ahm^{-2} of capacity value for 100 μm of side length. At 600 μm of side length the capacity value is 68,00 Ahm^{-2}. Side length increase implies an increasing of the maximum distance of the most distant ions to the collectors positions and the distance between the collectors and the thickness of the separator decrease. The increasing of maximum distance implies higher paths for charge movement (electrons and ions), leading to ohmic losses and a reduction of the capacity value. In the range of lengths from 100 μm to 600 μm it is observed an increasing of maximum distance from 200 μm to 1200 μm (Figure 2 (c)). Increased side length leads to a decreasing thickness of the separator (smaller distance between the collectors) and the ionic flow is facilitated through the separator as shown in Figure 2 (c). This effect leads to a gain in the capacity value. In the case of a side length from 100 μm to 600 μm, the losses of capacity value associated to a high maximum distances, are larger than the gains of capacity value associated a lower distance between collectors due to the lower thickness of the separator. The inverse effect occurs in the range of side lengths from 20 μm to 100 μm. The maximum distance is decreased, leading to a decrease of the ohmic losses. Further, the thickness of the separator and the distance between collectors are increased. It is concluded that the gains associated to the decreasing of maximum distance, thickness of separator and distance between the collectors are an important contribution for increasing the capacity value of battery. The optimal value of side length for the square frame geometry, obtained by Quadratic Regression Polynomial using Least Square Method, as illustrated in Figure 2 (b), is around 88 μm, leading to a capacity value of 189,40 Ahm^{-2}. Finally, it was compared the capacity value of two the square frame and rectangular frame geometries with the same maximum distance, distance between of collectors and thickness of the separator. Both geometries present the same capacity value of ~186,00 Ahm^{-2} at 500C. It is thus concluded that the same capacity is obtained using different geometries if the same maximum distances, distance between collectors and thickness of the separator are maintained.

CONCLUSION

The choice of battery geometry is important to improve the battery performance and allows to optimize the available space and shape in portable technologies where these batteries are applied. When the same area is maintained for all components, it should be taken into account the influence of geometrical parameters such as maximum distance, thickness of the separator and distance between collectors in the final balance of capacity value of the battery. In this work, the capacity value of the battery is evaluated as a balance between gains and losses of capacity value associated to geometrical parameters. When the geometrical parameter (side length of a square frame) is optimized according to the area, a higher performance at high discharges rates is obtained with respect to a conventional battery. Maintaining the same area for all components, the square frame geometry improves around 305,42 Ahm^{-2} the capacity value in comparison to the conventional geometry for high discharge rates (330C).

ACKNOWLEDGMENTS

This work is funded by FEDER funds through the “Programa Operacional Factores de Competitividade—COMPETE” and by national funds from FCT—Fundação para a Ciência e a Tecnologia, in the framework of the strategic project Strategic Project PEST-C/FIS/UI607/2014, project F-COMP-01-0124-FEDER-022716 and grant SFRH/BD/68499/2010 (C.M.C.). The authors also thank funding from Matepro – Optimizing Materials and Processes, ref. NORTE-07-0124-FEDER-000037, co-funded by the “Programa Operacional Regional do Norte” (ON.2 – O Novo Norte), under the “Quadro de Referência Estratégico Nacional” (QREN), through the “Fundo Europeu de Desenvolvimento Regional” (FEDER). F. Miranda was also supported by Portuguese funds through the CIDMA - Center for Research and Development in Mathematics and Applications, and the Portuguese Foundation for Science and Technology (“FCT - Fundação para a Ciência e a Tecnologia”), within project UID/MAT/04106/2013.

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