Comparison of anode materials for the optimization of the Lithium-ion batteries in terms of Higher Charging Capacity

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Abstract: In this research work an effort has been made applied for selecting the right anode material for the Lithium-ion batteries. For finding which material is the best in terms of the charging capacity an optimization technique using the mathematical model has been utilized. Through the utilization of the model, the charging capacity of the materials have been calculated and utilized for our research work. Through the optimization technique it has been found that the Silicon material has obtained higher charging capacities i.e. 5154 mAh/g as compared to graphite as an anode for the Lithium-ion batteries.

Keywords: Charging Capacity, Anode, lithium-ion batteries, Mathematical model

HIGHLIGHTS

- Mathematical model equations has been utilized for the specific capacity for the anode materials.
- Both the graphite and silicon material has been analyzed.
- The result has proven to be helpful in selecting the right material for the anode for the selection in the Lithium-ion batteries.

I. INTRODUCTION

With an increase in the utilization of the storage capacity through numerous methods the world need a viable solution for sustainability. The need for energy storage has made the world come up with new materials upgradation. These upgrades are important for making sustainable solutions. In the field of the Lithium-ion batteries, the new materials includes the silicon in the anode side electrode in the Lithium-ion batteries for the cathode as $LiMnO_2$. Silicon materials find its application in the field of solar cells, optical fibres, silicones and also in silicon chips, these technologies find multiple usage of the material and also its alloys for the engineering applications. Yang et al [1] did the multiscale design of the silicon/carbon composite anode material and the authors focused on the review for the various materials and how the materials are behaving at molecular levels including the nanoscale and microscale and the authors focused on the modifications, control and constructions for these materials. Dang et al [2] studied the effect of the coating strategy for the lithium-ion materials, the coating provides excellent ionic and electronic conductivity, elastic performance, making it more stable as compared to non-coating materials, making them significant for the Lithium-ion batteries. Zhang et al [3] worked on the improvement for the performance of the Lithium-ion batteries through the micro sized silicon particles coated with nano ZnS anode materials and remarkable results were published with the discharge specific capacity of 1540 mAh/g after the 200 cycles of charge – discharge. Li et al [4] silicon coating exhibits higher reversibility and outstanding cycling stability as compared to the other materials. Kim et al [5] studied the effect of the new types of silicon materials composed with the carbon composite and through the utilization of the chemical vapour deposition method the materials improved its electrical conductivity. Li et al [6] discussed the importance of various combinations of anode materials in which the SiOx based anode materials along with the combination of second phase compounding, prelithiation and electrolyte additive optimization. Finally, the authors emphasize the increase in electronic conductivity. Yuan et al [7] investigated the carbon material for the lithium-ion batteries and discussed the importance in terms of the charge storage as the carbon has the large specific surface area and having higher values of electrical conductivity. The authors emphasized the importance of one-dimensional carbon material and graphene as substitute materials for the anode materials and proven to be applicable for high range of electrical appliances. Tian et al [8] discussed the advantage of reversible lithium plating for fast charging capacity in low temperature lithium-ion batteries. The authors also emphasized on the PWFC plating weak fast charging keeping the charging rate with larger amplitude throughout the charging- discharging cycles. Jo et al [9] discussed the anode free batteries as the next generation of power storage, the authors focused on the impingement of excess lithium on the cathode and reducing on the anode. The authors also contributed the significance of the electrolyte modification and the utilization of the solid electrolyte interface. Authors emphasized the use of lithium metal achieving the charging capacity as high as 3860 mAh/g. Ref the above research findings an idea for the generation of the specific capacity for the graphite and silicon using the mathematical model has been generated through the equations and also the effect of the temperature on the specific capacities have been described in the research work.

II. LITERATURE REVIEW

In this research work Silicon has been used as the substitute material in place of the graphite as the anode material. Silicon has been promising material with its large energy gap i.e. 1.1 eV compared to the other materials. Lithium Metal with the combination of the manganese oxide has been the promising in terms of the stability of the cathode materials for the cathode. In this research work emphases has been given on the combination of the anode and the cathode with the change in the anode material. The substitute for the graphite with the silicon has been utilized for the research work. The classification for the anode materials has been described in the Table 1.

Table 1 Classification of anode materials

Sr. No.	Material	Properties
1.	Graphite	Having capacity ranges 372 mAh/g with low cost and good energy density.
2.	LTO	Used in various automotive applications and can handle higher temperature regions with temp ranging from 50-70^{o}C.
3.	Hard Carbon	Has greater storage capacities
4.	Tin/Cobalt alloy	Consumer Electrons
5.	Silicon Carbon	Has approximately 74 mAh/g the energy density and provides longer life cycle upto 5000 mAh

III. RESULTS AND DISCUSSION

a. Mathematical Relation between the specific capacity and the amount of Lithium-ion Intercalation

Table 2 Value for the Graphite as anode material during the intercalation with Lithium

Sr. No.	Parameter	Value	Units
1.	Molar Mass of Graphite	12	g/mol
2.	Molar Mass of LiC_6	72.94	g/mol
3.	Number of Faradays	1	-
4.	Faraday's Constant	96485	c/mol

$$C_{theoritical} = \frac{nF}{M_{LiC_6}} \quad \text{Eq.1.}$$

Through the insertion of the data through the tabulated values given in table 1. The theoretical value for the Specific capacity for the graphite materials i.e. 1322 mAh/g.

Table 3 Value for the Silicon material during the Intercalation with Lithium

Sr. No.	Parameter	Value	Units

1.	Molar Mass of Silicon	28.0855	g/mol
2.	Molar Mass of $Li_{15}Si_4$	216.442	g/mol
3.	Number of Faradays	15	-
4.	Faraday's Constant	96485	c/mol

$$C_{theoritical} = \frac{nF}{M_{Si}} \quad \text{Eq.2.}$$

Through the insertion of the data through the tabulated values given in table 1. The theoretical value for the Specific capacity for the graphite materials i.e. 5154 mAh/g.

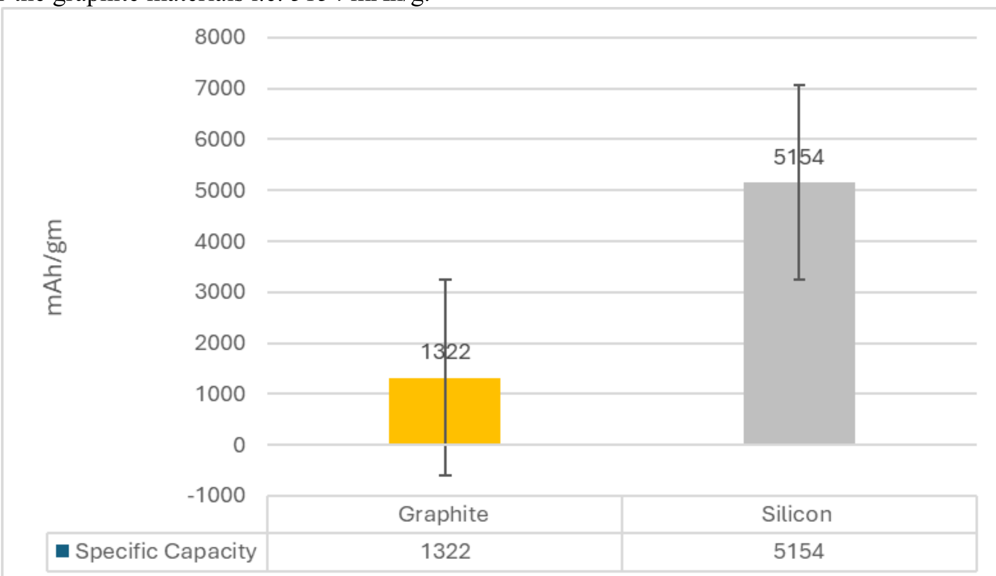

Fig.1. Specific Capacity for the anode materials

Figure 1 shows the specific capacity for the anode materials for the graphite and silicon. Through the results generated through the utilization of the mathematical model equation the higher value has been generated for the silicon material i.e. 5154 mAh/g which is almost approximately 300 % rise in the initial value for the Graphite. Through these higher values the material substitution can be utilized in the Lithium-ion batteries.

b. Mathematical Relation between the specific capacity and temperature at different temperature values

$$C_T = C_{T_{ref}} \times e^{\left(-\frac{Ea}{k}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)\right)} \quad \text{Eq.3.}$$

Through mathematical calculation when we substitute the value for the graphite materials the C_T at 25°C is 3500 mAh and with 40°C is 4224.5. The values of C_T for the silicon material at 25°C is 4200 mAh and with 40°C is 6115 mAh respectively. The higher temperature values for the graphite materials obtained are due to the enhanced kinetic energy of the lithium-ions intercalation at higher temperatures. Similarly for Silicon Materials the main reason for the higher values of the specific capacity are due to the overpotentials in the silicon as compared to graphite.

IV. CONCLUSIONS

- Through the utilization of the mathematical model Silicon material has the higher specific capacity value obtained i.e. 5154 mAh/g.
- Through research it has been found that the Silicon has the higher activation energy leading to more pronounced increase in the specific capacity with respect to temperature.
- Temperature plays a significant role, with the increase in the temperature there is an increase in the specific capacity and these values are higher for the silicon material i.e. 6115 mAh at 40°C.
- Silicon material has a large energy gap i.e. 1.1 eV which makes its operate at higher temperature ranges as compared to other materials such as graphite. These findings will make the silicon material as anode more attractive.

Acknowledgement: We sincerely thank our Honorable Vice Chancellor, Prof. (Dr.) Gadangi Indira for her invaluable inspiration and support in completing our research. Her provision of essential resources has been instrumental in the successful execution of this work.

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