Study of Electrochemical performance of LMO electrode for variable thickness using 1-D Modelling and simulation

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SUBMITTED IN PARTIAL FULFILMENT OF THE REQUIREMENTS

FOR THE AWARD OF THE DEGREE

OF

MASTER IN SCIENCE

IN

PHYSICS

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DECLARATION

I, Harsh (2K21/MSCPHY/17) and Bhoodev(2K21/MSCPHY/11) hereby certify that the work which is presented in the Dissertation-II entitled in fulfillment of the requirement for the award of the Master in Science in **Physics** and submitted to the Department of **Applied Physics**, Delhi Technological University, Delhi is an authentic record of my own, carried out during a period from January 2023 to May 2023 under the supervision of **Dr. Amrish Kumar Panwar and Dr. Pawan Kumar Tyagi.**

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CANDIDATE'S DECLARATION

I, Harsh (2K21/MSCPHY/17) and Bhoodev (2K21/MSCPHY/11), students of M.Sc. Physics, hereby declare that the project Dissertation titled "Study of Electrochemical performance of LMO electrode for variable thickness using 1-D Modelling and simulation" which is submitted by me to the Department of Applied Physics, Delhi Technological University, Delhi in partial fulfillment of the requirement for the award of the degree of Master in Science, is original and not copied from any source without proper citation. This work has not previously formed the basis for the award of any Degree, Diploma Associateship, Fellowship or Other similar title or recognition.

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Date: 31 May 2023

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CERTIFICATE

We hereby certify that the project titled "Study of Electrochemical performance of LMO electrode for variable thickness using 1-D Modelling and simulation" which is submitted by Harsh (2K21/MSCPHY/17) and Bhoodev (2K21/MSCPHY/11), Department of Applied Physics, Delhi Technological University, Delhi in partial fulfillment of the requirement for the award of the degree of Master in Science, is a record of the project work carried out by the student under my supervision. To the best of my knowledge this work has not been submitted in part or full for any Degree or Diploma to this University or elsewhere.

Place: Delhi **Dr. Pawan Kumar Tyagi**

Date: 31 May 2023

Dr. Amrish Kumar Panwar

SUPERVISOR

ABSTRACT

In this study, the 1-D (one dimension) simulation for a Lithium-ion battery (LIB) has been performed by using the multi-physics software for better electrochemical performance of the battery. The cathode material chosen for the simulation is $LiMn_2O_4$ (LMO), along with $LiPF_6$ as electrolyte and lithium metal as anode. The experimental data and published work were used to acquire the various input parameters used in the model formulation. The variable thicknesses of the cathode material LMO has been changed as 50um, 75μm, 100μm, 125μm,150μm and 175μm while the thickness of separator and anode material is kept constant during simulation. The discharge curves for variable thickness at different C rates such as 0.5C, 1C, 2C, and 4C have been obtained using the simulation. The findings of this study may be useful in optimizing the electrode thickness for the required capacity of a lithium-ion battery based on its use.

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ACKNOWLEDGEMENT

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Harsh

Bhoodev

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CHAPTER-1

INTRODUCTION

1.1 Background

As the Population increasing with times, the demand of energy also increasing and to meet this demand various source of energy like coal, crude oil and natural gases etc. are being used but these type of energy sources are non renewable and will diminish in the near future. [1]These type of sources when used then they also produces the various polluting substances and green house gases which cause the various problem for ecological balance of earth.[2] To overcome these problems the research on various renewable source happening across the world . Wind energy, solar energy, water energy and geothermal energy etc. these are the some of the type of renewable energy. Batteries are also one type of renewable energy source which can be recyclable and efficiently store the energy.[3]

Air pollution and the global warming can be abolished by using the batteries in vehicles and in other devices where the Where the need of energy storage is required.[4] Batteries are lightweight and have high capacity to energy storage and when they are used in the electrical vehicle then the pollution is not produced.[5] These batteries are versatile source of energy which can be stored in very small space and used in devices like smartwatches. Regardless of various advancements in energy storage devices, there is a deficit of proper energy storage techniques which can be only abolished and reduced using the batteries.[6]

1.2 Batteries

Batteries are electrochemical devices that have capacity of storing and releasing energy, which are allowing the electrical supply to be load-balanced. A battery is defined as a collection of cells that are connected in all in parallel and series, or all combinations. An electrochemical cell consists of an anode and a cathode that are separated by a separator and have electrolytes filled in the pores electrode. Other than energy production uses, rechargeable batteries are seen as an reliable power source for electric vehicle utilisations and have been focussed capably since they were originally given a long time ago.[7] To be a viable alternative to petroleum based energy, a battery must fulfil a few requirements in terms of cost, health, energy, and power. Batteries have many types on the basis of chemicals but on the basis of electrochemical reversibility there are two types only which are primary and secondary types.[8]

1.2.1 Types of Battery

Batteries have been categorised into two types:

1. Depending on their electrochemical reversibility
    a. Primary Battery
    b. Secondary Battery

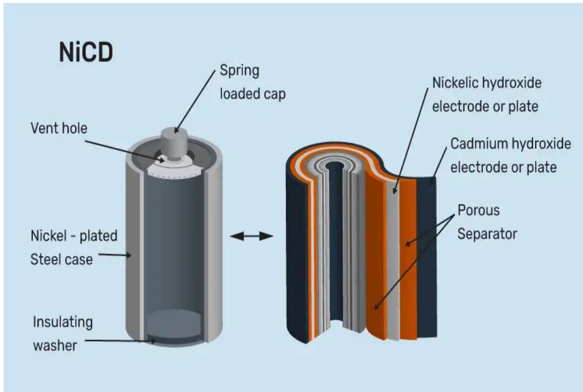
Primary Batteries

Primary batteries, often known as throwaway batteries, are energy storage devices that are not able to be recharged.[9] They are taken in consideration for one-time usage only and cannot be replenished once there energy exhausted. Primary batteries are extensively used in compact electronic gadgets, home appliances, and various other uses that require a short-term power supply. These batteries come in a variety of sizes, including D, C, AA, AAA, PP3, and coin cells.[10]

Secondary Batteries

Secondary batteries, generally referred to as batteries that recharge and are a form of battery that can be both recharged and reused. Primary batteries, on the other hand, are thrown away and cannot be recharge.[11]

Secondary batteries have ability to transfer and store electrical energy during charging and releasing it when required during discharge. Because the chemical processes inside the battery are able to be reverse numerous charging as well as discharging cycles are possible. Secondary batteries have the benefit of being reused, making them less expensive and more ecologically friendly than main batteries. They do, however, have limits, such as a limited lifetime and discharge by themselves over time.[12] Second batteries can be utilised when primary batteries is too expensive or impracticable to use for heavy drain applications. Secondary battery supporting limited capacity batteries used in small electronics such as cordless phones, laptop computers, and mobile phones. Secondary batteries for hybrid or electric cars with significant power consumption, as well as load generation to manage power supply. Secondary batteries include Ni-Cd batteries, lead-acid batteries, lithium-ion batteries, and so on.[13]



(a) **(b)**

Figure 1.1. (a) Ni-Cd Battery, (b) Li-ion Battery

Table 1.1. Theoretical data about different batteries[3]

Batteries	**Li-ion**	**Pb -acid**	**Ni-Cd**
Lifetime/cycle	410~1200	210~500	2000
Working Potential (V)	3.6/3.85	1.0	1.1
Gravimetric energy densityor Specific energy (Wh/Kg)	100 -265	40-60	40-70
Volumetric Energy densityor energy density (Wh/L)	250-694	100	50-150
Specific Power (W/Kg)	250-340	90-120	150
Self-Discharge (% permonth)	2.5-5%	3-5	10
Charge/ Dischargeefficiency (%)	80-90	90-99	70-90
Weight	Light	medium	Heavy

Li-ion batteries are being arguably the most remarkable rechargeable battery and have been consequently gotten a lot of attention in recent years. They are currently the most important part of the entire lightweight electrical energy source for accessible electronic devices, primarily utilised in mobile phones and PCs. Li-ion batteries have been viewed as an entity to be considered when it comes to computerised electronic systems from over twenty years ago, around at the same time that lithium-ion cells were marketed.[14] As one can notice from his or her daily activities, the increasing use of flexible gadgets necessitates improved Li-molecule cells. For example, powering the mobile phone with growing functions less frequently than the continued phone will cope with the concept of one's life. Another fast increasing market of Li-ion batteries is hybrid and electric vehicles, which require innovative Li-ion cells with outstanding power, high charging rate, strong cutoff, and a lengthy life, in addition to enhanced security implementation and lower cost.[15]

1.3 Working of Battery

The cathode, electrolyte, and anode are the three essential components of a rechargeable battery or cell, as depicted in Figure1.2. The degree of attraction or affinity that different metals and their compounds have for the electrons varies. An electrochemical potential is created whenever two different metals and compounds made up of them are combined by means of an electrolyte, a medium.[11] The cathode loses electrons and becomes weakened electron affinity, while the anode drops electrons thus becomes negative in charge due to its higher affinity for electrons. Because of the electrochemical potential, ions that are positive travel from the negatively charged anode to the other electrode through the electrolyte. Electrolytes' primary goal is to prevent electrons from passing through them and allow ions to pass through them. When the ion moves from the anode to the cathode, the neutral charge distribution is disrupted, so electrons move through the external circuit to restore it. A capacitive charge immediately builds up in the absence of an external circuit to prevent the battery from draining. A capacitive charge immediately builds up in the absence of an external circuit to avoid the battery against draining. To avoid short-circuiting, an electrolyte separator is inserted between the two terminals of the battery.[16]

The overall reaction during discharging can be represented as:

Anode: LiC6 ⟶ Li+ + C6 + e-

Cathode: LiCoO2 + Li+ + e- ⟶ LiCoO2r

The overall reaction during charging can be represented as:

Anode: Li+ + C6 + e- ⟶ LiC6

Cathode: LiCoO2 ⟶ LiCoO2 + Li+ + e-

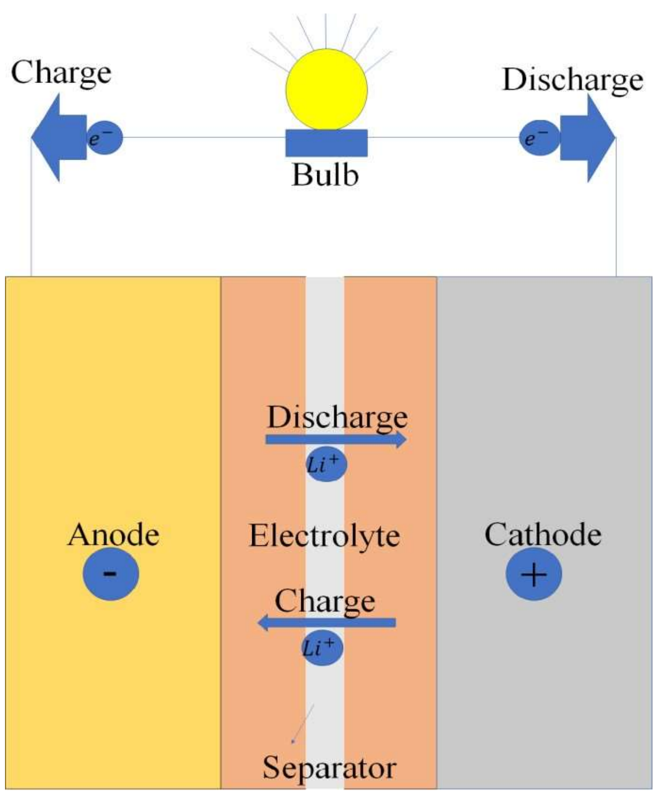


Figure 1.2. Battery diagram

1.4 Advantages of Li Ion Battery:-

The following advantages distinguish LIBs from other battery systems, including:

- a wide temperature range of operation
- a high energy density
- excellent cycling performance
- a relatively low self-discharge
- Lithium-ion batteries have a prolonged cycle life and an extended shelf-life.
- They require minimal maintenance.

1.5 Disadvantages of Li Ion Battery:-

- The use of the protection circuit is essential and required to safeguard against thermal runaway in lithium-ion batteries.
- Elevated voltage and temperature conditions may lead to the potential damage and failure of li-ion batteries.
- Rapid charging is not feasible and hard when operating below 0°C (32°F) temperatures.
- Adequate adherence for transportation regulations is necessary when shipping lithium-ion batteries in larger quantities.

1.6 Cathode

The cathode is a crucial part of a battery, especially in lithium-ion batteries. During discharge, reduction processes occur at this electrode, storing and receiving positive ions or electrons. The following qualities are necessary for materials used as cathodes in batteries:[17]

Table 1.2. Different cathode materials and their properties value

Cathode Material	Energy Density (Wh/kg)	Capacity (mAh/g)	Cycle Life	Cost
Lithium Cobalt Oxide (LCO)	150-200	150-200	300-500	High
Lithium Manganese Oxide (LMO)	100-150	100-150	500-1000	Low
Lithium Nickel Manganese Cobalt Oxide (NMC)	150-200	100-150	500-1000	Medium
Lithium Nickel Cobalt Aluminium Oxide (NCA)	200-250	100-150	500-1000	Medium
Lithium Iron Phosphate (LFP)	100-120	100-150	1000-2000	Low

Cathode materials have the following characteristics:

- As oxidising agent is efficient.
- operating voltage is useful and in range
- Ease of manufacture
- Stability when in touch with the electrolyte
- Low cost

Lithium-ion batteries employ a variety of cathode materials, including lithium cobalt oxide ($LiCoO_2$), lithium nickel manganese cobalt oxide (NMC), lithium iron phosphate ($LiFePO_4$), and lithium manganese oxide ($LiMn_2O_4$). Each material has an own set of attributes and trade-offs, allowing battery producers to adapt their features according to particular application needs.in this study we aim to improve lithium manganese oxide ($LiMn_2O_4$) material in order to increase lithium-ion battery energy storage capacity, lifespan, safety, and performance as a whole.[18]

1.7 Lithium Manganese Oxide (LMO)

$LiMn_2O_4$ which is widely known as lithium manganese oxide, is one of the cathode materials that exhibits excellent structural stability throughout the charging and discharging process. The Sanyo firm which originally commercialised LMO batteries in 1975, made these batteries one of the earliest Li-ion batteries to be marketed commercially. $LiMn_2O_4$ possesses a spinel structure which enables the three-dimensional intercalation in them. This leads to lithium ion to get inserted into the cathode material in three different ways. The $LiMn_2O_4$ spinel drives demonstrate a lack of longevity and irreversible capacity loss at the elevated temperatures.[4] Lithium Manganese Oxide ($LiMn_2O_4$) is a cathode material often utilised in the rechargeable lithium ion batteries. LMO is thought as a good cathode material due to its vast availability, ecologically harmless and the low price, ease of fabrication, and high specific theory.[13]

A standard LMO battery has the 3.7 V operational voltage. Faraday's first law in electrochemistry, which specifies that 1 gram equivalent weight of any substance would give 96487 coulombs (or 26.8 Ah), may be used to readily compute a material's theoretical capacity. When contemplating the synthesis of the novel materials, this might be quite beneficial. It is simple to determine if this material is capable of competing in regard to specific capacity against the currently available electrode materials. The equivalent molecular weight (M), which is of $LiMn_2O_4$ is 180.8 g/mol, resulting in its theoretical capacity is: 26.8/180.8 = 148 mAh/g. Similarly, if the entire charge/discharge range is used, the theoretical capacity for the $LiMn_2O_4$ cathode may be found to be 285 mAh/g.[18]

LMO batteries have a slightly higher voltage than the NMC batteries, which have 3.6 V under load and a specific capacity of 170 mAh per gram. However, LMO batteries have a lower specific capacity in comparison to NMC batteries.

The key problem in dealing with the batteries in the future is achieving the largest capacity while remaining modest in size. There are several elements that influence the battery capacity, including the sort of active material used, the composition that makes up the sheet, and the degree of thickness associated with active material utilised during the electrochemical method. As a result, the increment in thickness of the active chemicals on the electrodes per unit area is essential for ensuring to effectively maximise the battery's capacity.[10] However, the addition of an enormous amount of active material may not give required results, so the quantity of active material engaged in the electrochemical process must be optimised. This study will also discuss the changes in the thickness of active materials used in the construction of battery cells.[5]

Advantages of LMO:

- vast availability
- ecologically harmless

- the low price ease of fabrication
- High specific capacity

Disadvantages of LMO:

- Manganese Dissolution
- Limited High-Temperature Performance
- Voltage Fading

The theoretical research on lithium-ion battery cells using LMO-based cathode materials have been conducted. As a result, a model has been developed via the simulation and provided the initial values. A one-dimensional (1-D) model is created by varying thickness of LMO cathode. Finally, the optimised thickness was determined for optimum electrochemical performance, and the polarisation effect, charging and discharging voltage, and other factors were explore.[2]

CHAPTER - 2

LITERATURE REVIEW

Ian S. Huber, 2017 In this research paper the authors of this article used a Multiphysics programme called COMSOL to create a one-dimensional model of lithium-ion batteries. This model generates the graphs of the battery's electrolyte content, voltage, and release rates over time. To further understand the model, they varied the volumetric divide (porosity) of the positive and negative electrodes, the electrical conductivity of the positive and negative electrode the dispersal coefficient of the battery separator, and the rate of the discharge flow to observe the effects on the concentration, voltage, and discharge rates. They discovered that the volumetric component of the two anodes, the electrical conductivity at the positive anodes, and the release current all have an effect on focus and voltage, whereas dissemination had no effect on discharge rates. Negative terminal conductivity had no effect on any of the dependent variables. With these findings, better understanding of the battery models may be gained in anticipation of the potential creation of successful lithium-ion batteries for commercial usage.[12]

Xiao, Xinran, Huang and wei, Xiaosong. 2010 in this research article tell that the pressure within the battery when charging and discharging. The separator is a porous membrane that is put between either indirect or direct electrodes in order to avoid physical contact and enable ionic transportation while preventing physical contact and enabling ionic transport. The electrode size and thermal conductivity of the two battery parts fluctuate as a result of the lithiation and de-lithiation, which may generate pressure across the separator. Based on this review, there is no means to verify the pressure within the battery till then. As a result, the cell's differential pressure assessment is carried out in a constrained multiple scales element. A little damage on the separator is normal owing to the electrode's molecules under pressure. Surface roughness is greater in curved sections than in normal dividing areas. As a result, increased difficulty is encountered in the separator's tight space. The stress condition and dimension in the separator are determined by particle size, packaging, and battery cell dimension. In the event of a loose particle pattern, there is an intense pressure in the separator, but in the scenario of a closed particle arrangement, there is a compressive stress under normal pressure and adequate pressure within the separator.[18]

Rahul Deb Pal, 2015 in this paper the authors of this research simplified a few boundaries of the battery model and validated the results with the charge-release bent by exploratory result. Their research findings are important in determining the conditions that maximise battery use. In this testing, the battery was charged and released several times at a slow rate of 0.04C at ambient conditions in order to achieve a constant limit. Following that, galvanostatic recharging and discharging at a 1C rate with voltages ranging from 2.8 V to 3.8 V at 100, 300, and 400 degrees Celsius. Compare these results to the one-cell full-cell model of COMSOL Multiphysics version 5.0 includes a layered isothermal temperatures lithium-particle cell model. This might be employed in the design of electrical devices and battery board frameworks.[14]

A. Rozenblit, 2021 The researchers utilised Comsol Multiphysics to perform simulations for various atom diameters of $LiMn_2O_4$ used as the cathode in Li4Ti5O12

(LTO)- (LMO) batteries . The findings show that higher numbers of tiny particles at uniform cathode material stress and accurate current density throughout electroactive area may allow higher flows to be implemented due to compensating greater dynamic surface area/unit volume, which reduced the local current its thickness at the LMO crystal connection with known electrolyte. These findings emphasise the relevance of morphology and PS in battery designs, notably in the LTO-LMO architecture.[1]

Satish Kumar B. 2014 reviewed an overview of the developing cathode material being developed for usage in electric cars. Integrated cathode frameworks are a one-of-a-kind combination that offers advantages over a cathode comprised of sole material. The benefits include an extended cycle life and a lower cost. As a result, lithium-particle cells that use spinel as the cathode component may be particularly challenging in auto incentive usage applications wherever battery durability longer than other operating temperatures is critical. Spatial adjustments have been used successfully in various cathode schemes to further expand cathode molecule toughness and credibility and to further increase cell health execution and will most likely remain a portion of single-part or integrated frameworks. Progress in developing better techniques to enhancing strength, wellness, and security is going to be made. Newer synthetics will be anticipated to address the energy demands of PHEV or BEV usage in the long run. Furthermore, rapid charging has shown to be more effective in addressing the difficulties of the modern way of life. Integrated frameworks can form the middle of the primary cathode, which is particularly well-equipped for accusing of high calibre. Currently, Li-rich mixes and Li-sulphur structures offer exceptional assurance; nevertheless, intermediate improvements using some of the strategies portrayed here may be beneficial, and instances discovered regarding collecting and shielding cathode frameworks will most likely function. Otherwise, technological developments may result in less priced cathode components. Cathode methods of assembly and covering may be viable. Otherwise, technological developments may result in less priced cathode components.[15]

Cai, Long and Ralph E. White. 2011 made an electrode in presence of pulse and absence of pulse which was providing the output with the same amount of power supply and analysed the thermal conductivity. They used different C rates to do this experiments like they eliminated the battery for 3000s at different rates of C/2 and 3C and wait for the voltage to drop to 2.5V. They reached to a conclusion that now cell was performing better in temperature-separated state, i.e., isothermal state has lower excretion rate than the adiabatic state. This is due to the factor that diffusion coefficient of binary electrode is high and it results in the sudden increase in the temperature of cell at 1C and it gradually increases the diffusion limits for isothermal than adiabatic conditions. They also came to the conclusion that cell may collapse due to rise in temperature because of excess heating.[11]

Zhang, Sheng Shui. 2007 figured out some various kind of separators which we can use in a lithium ion battery having electrolyte in liquid state. We segregate the battery divider which is separator based on the material they are made up of and their shape or structure into three groups. First is membrane which is made up of polymer and has microporous structure, second is mats made up of non-woven fabric and the third one is membranes which are made up of inorganic composites. Above mentioned all three separators exhibits distinct properties such as membrane made up of polymer and has microporous structure has slim structure and insulating properties at high temperature, fabric material which is untreated identified by minimal price and more porosity whereas in membranes which are made up of composites have exceptional stability with high range of temperature and phenomenal moisture properties. Basically in this particular review modifications done in batteries like battery divider, features tell us about the batteries' efficiency and the safely environment.[6]

Sumitva De 2013 made a model system by using comsol in which they can optimize design characteristics for electrodes which are porous, simulatneously and they were being used very commonly in batteries which are very advanced in nature like lithium ion. After seeing the results we observed a phenomenal improvement especially in the specific energy which was taken from the lithium-ion battery when we optimized the parameters of design simultaneously. They also used the Gaussian process so that model can be optimized simultaneously and can be monitored successfully. Optimization of only one parameter technique was considered so that they can easily conclude the variation and can explain the reasons of variation. Only in that condition this can be used successfully. Thickness ratio of cathode to anode was kept constant but in case of anode, they varied it's thickness based on the optimization boundation.[4]

CHAPTER -3

MODEL DEVELOPMENT

3.1 Introduction

COMSOL is the computational modelling programme with restricted components that is used for solving numerous PDEs in the fluid stream, Acoustics, and solid-state mechanics. It is a commercialised restricted component programming package designed to solve a wide range of real-world anomalies. Given the increased usage of this item in perceptive electrochemistry, the makers intend to revisit its significance and practical application in this sector. The programme is sufficiently versatile to accommodate many PDEs in one region simulation. Furthermore, to summarise PDEs which can be performed for particular issues, COMSOL has a basic library of preconfigured PDEs for specific uses (heat, liquid components, diffusion, and more), in addition to summarise PDEs which can be performed for specific difficulties. COMSOL Multiphysics software provides a framework for simulating any physical phenomenon by using ordinary and partial differential equations (PDEs). This programme is capable of running or installing on practically all systems, including Linux, Mac, as well as all variants of Windows.[3]

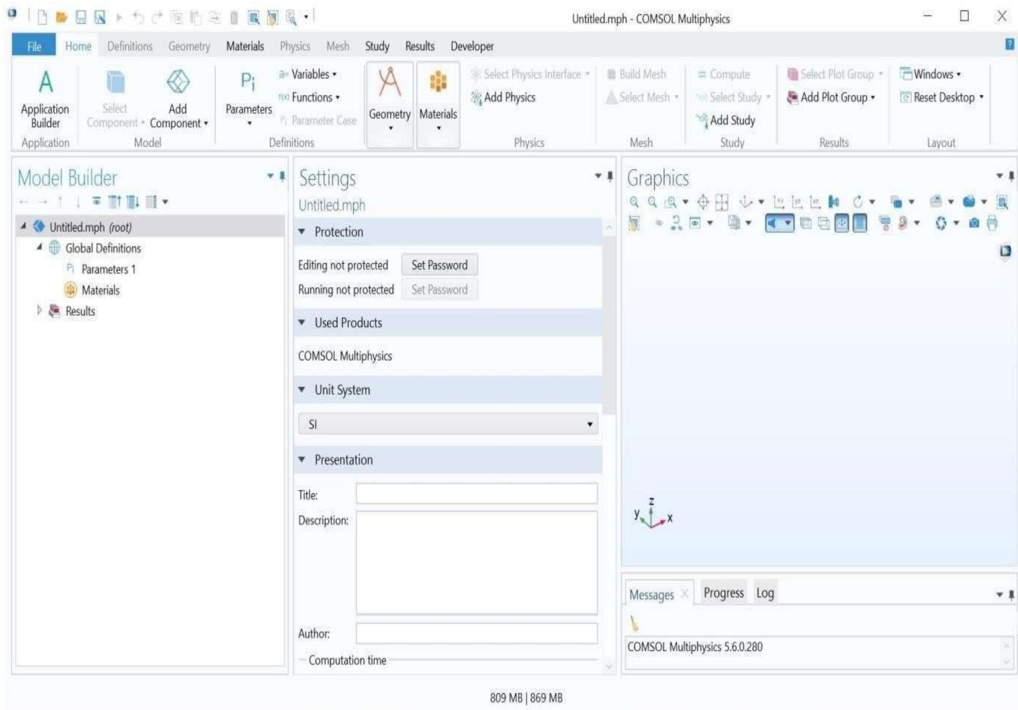


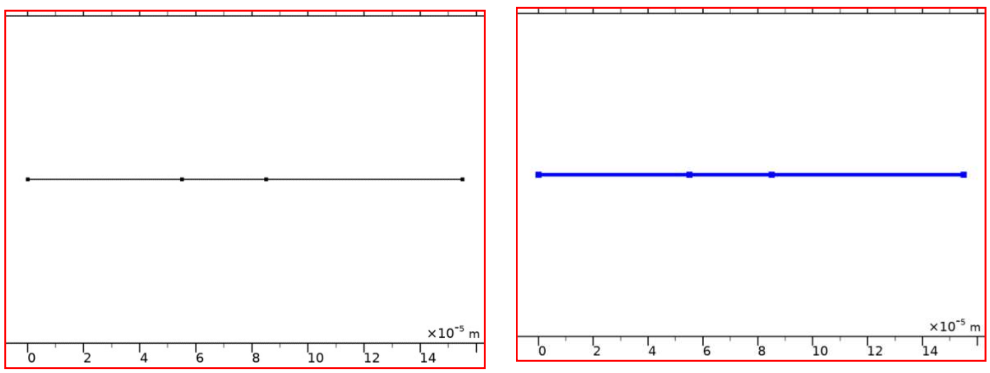
Figure 3.1. COMSOL Multiphysics Software Layout.

3.2 Our Model

Materials: The cathode material chosen for the simulation is $LiMn_2O_4$ (LMO), along with $LiPF_6$ as electrolyte and lithium metal as anode. Also the experimental data taken from various literatures.

Modelling of Battery cell: In this work, we develop a 1-D geometry of lithium-ion-battery to optimize the cathode thickness for material $LiMn_2O_4$ using COMSOL Multi physics software. For this purpose, six cells with different cathode thickness 50μm, 75μm,100μm,125μm,150μm and 175μm have been modelled of material $LiMn_2O_4$, and lithium-foil as an anode material and these two electrodes are separated by a polymer based porous separator of thickness of 50 μm. Pores are filled with electrolyte $LiPF_6$ in

1:2 EC : DMC (Ethylene Carbonate : Dimethyl Carbonate). The required electrode and electrolyte parameters for battery modelling are taken from the literature. These cells has been tested for various C rates such as 0.5C, 1C, 2C, and 4C and results have been obtained.[3]



(a) (b)

Figure 3.2. (a) 1-D model geometry of battery without electrolyte , (b) 1-D model geometry of battery with electrolyte

Steps for, building a 1D model of a lithium-ion battery using COMSOL

- Creating a one-dimensional lithium-ion battery involves making a positive electrode, an electrolyte separator, and a negative electrode with a current feeder, and then clicking the create all button.
- Select suitable anode, cathode, and electrolyte materials.
- Enter the material attributes into the model.
- Assign a Domain to each component.
- Each domain has its own set of boundary conditions.
- The mesh is now produced.
- Run model so that it simulates
- Analyse the findings to get the required data from the experiment.

CHAPTER – 4

PARAMETERS

4.1 Materials:

The cathode material chosen for the simulation is $LiMn_2O_4$ (LMO), along with $LiPF_6$ as electrolyte and lithium metal as anode. Also the experimental data taken from various literatures.

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In this work, we develop a 1-D geometry of lithium-ion-battery to optimize the cathode thickness for material $LiMn_2O_4$ using COMSOL Multi physics software. For this purpose, six cells with different cathode thickness 50μm, 75μm, 100μm, 125μm, 150μm and 175μm have been modelled of material $LiMn_2O_4$, and lithium-foil as an anode material and these two electrodes are separated by a polymer based porous separator of thickness of 50 μm. Pores are filled with electrolyte $LiPF_6$ in 1:2 EC : DMC (Ethylene Carbonate : Dimethyl Carbonate). The required electrode and electrolyte parameters for battery modelling are taken from the literature. These cells has been tested for various C rates such as 0.5C, 1C, 2C, and 4C and results have been obtained.

Table 4.1. Table for Parameters

Name	Value	Description
epss_filler_neg	0.026	Conductive filler phase volume fraction, negative
epss_filler_pos	0.073	Conductive filler phase volume fraction, positive electrode
i0_pos_ref	0.08[mA/cm^2]	Exchange current density at reference conditions, positive electrode
i0_neg_ref	0.11[mA/cm^2]	Exchange current density at reference conditions, negative electrode
epsl_neg	0.503	Electrolyte phase volume fraction, negative electrode
epsl_pos	0.63	Electrolyte phase volume fraction, positive electrode
C	0.1, 1, 2, 4	C-rate factor for the parametric study
Ks_neg	100[S/m]	Solid phase conductivity negative electrode
L_neg	100e-6[m]	Length of negative electrode
cs_neg_ref	14870[mol/m^3]	Reference concentration negative active electrode material
i_1C	17.5[A/m^2]	1C discharge current
L_pos	(175,150,125,100,75,50)e-6[m]	Length of positive electrode
Ds_pos	1e-13[m^2/s]	Solid phase Li-diffusivity positive electrode
cl_0	2000[mol/m^3]	Initial electrolyte salt concentration

cl_ref	2000[mol/m^3]	Reference electrolyte salt concentration
t_disch_stop	2000[s]	Discharge duration
t_charge_stop	2000[s]	Charge duration
csmax_pos	22860[mol/m^3]	Max solid phase concentration, positive electrode
csmax_neg	26390[mol/m^3]	Max solid phase concentration, negative electrode
T	298[K]	Temperature
brugg	3.3	Bruggeman coefficient
Ds_neg	3.9e-14[m^2/s]	Solid phase Li-diffusivity negative electrode
t_ocp	300[s]	Open circuit duration
cs0_pos	3900[mol/m^3]	Initial concentration positive active electrode material
L_sep	52e-6[m]	Length of separator
rp_pos	8e-6[m]	Particle radius positive electrode

CHAPTER-5

RESULTS AND DISCUSSIONS

Figures given below show the discharge capacity of $LiMn_2O_4$ cathode at different C rates and variation of these with the thickness of cathode. First we observe the voltage vs discharge capacity at thickness of 50μm for different C rates like 0.1C, 1C, 2C and 4C. C-rate basically tells us about the time battery takes to fully charge or discharge. 1C means battery can be completely charged or discharged in 1 hour. Similarly 2C means that battery can be completely charged or discharged in 30 minutes, 4C means that battery can be completely charged or discharged in 15 minutes.

5.1 GRAPH OF VOLTAGE V/S DISCHARGE CAPACITY AT VARIABLE THICKNESS

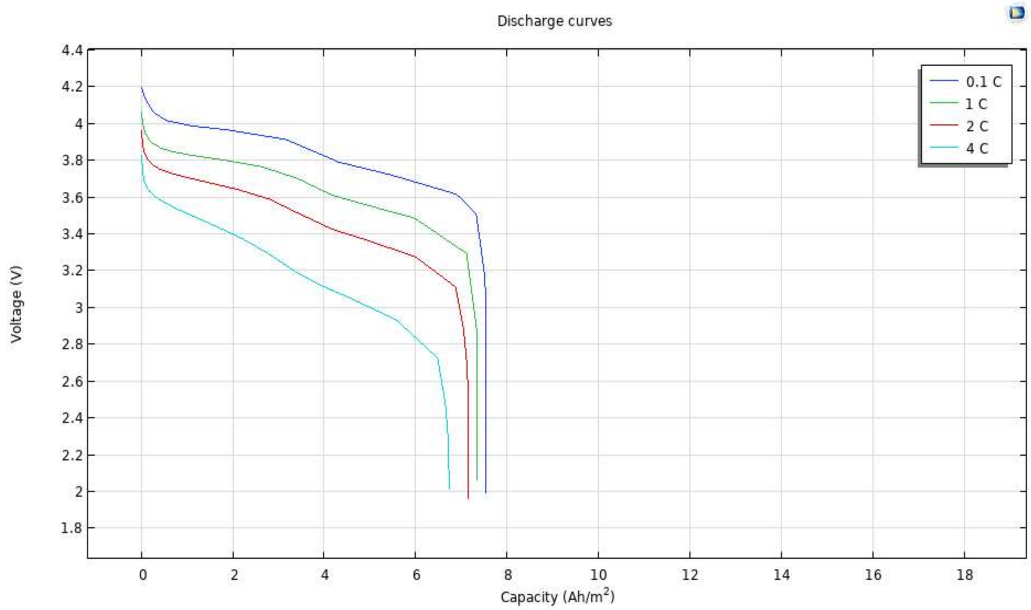

Figure 5.1 Electrode of thickness 50μ m

As we can see for cathode of thickness 50μ m voltage is different for different C-rates, voltage for 0.1C is 4.2, for 1C it is 4.1, for 2C it is 3.9 and for 4C it is 3.8. Discharge capacity is also different for different C-rates, discharge capacity for 0.1 C is 7.8, for 1C it is 7.75, for 2C it is 7.65, for 4C it is 7.45. So in this we can clearly observe that with the increase in C-rate discharge capacity is increasing. Let's observe this for other values of thickness. Further we will see how we will vary the thickness and the voltage vs discharge capacity will change

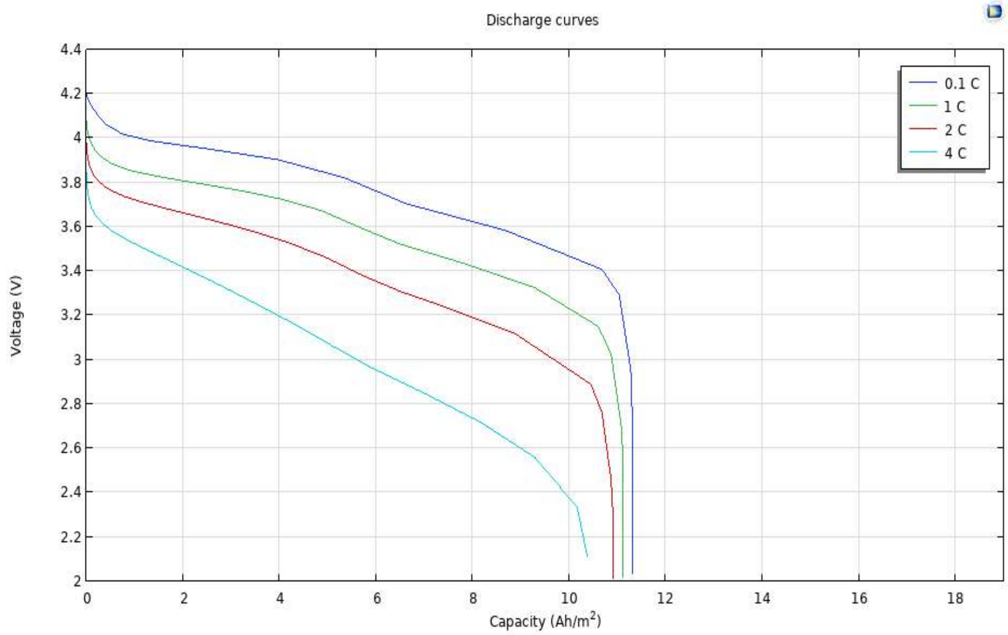

Figure 5.2 Electrode of thickness 75μ m

As we can see for cathode of thickness 75μ m voltage is different for different C-rates, voltage for 0.1C is 4.2, for 1C it is 4.1, for 2C it is 4 and for 4C it is 3.8. Discharge capacity is also different for different C-rates, discharge capacity for 0.1 C is 11.3, for 1C it is 11.1, for 2C it is 10.9, for 4C it is 10.3. So in this we can clearly observe that with the increase in C-rate discharge capacity is increasing. Let's observe this for other values of thickness. Further we will see how we will vary the thickness and the voltage vs discharge capacity will change.

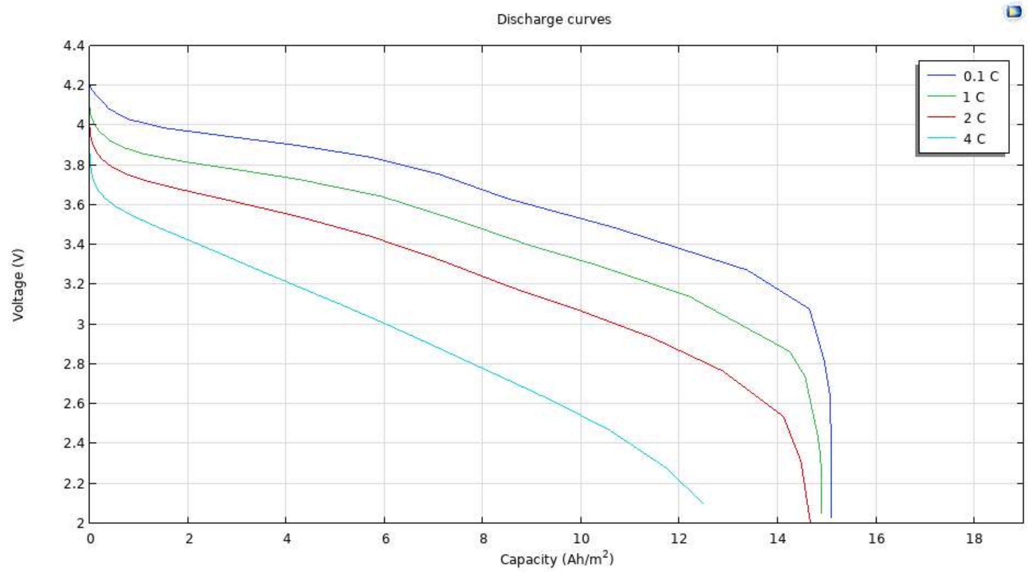

Figure 5.3 Electrode of thickness 100μ m

As we can see for cathode of thickness 100μ m voltage is different for different C-rates, voltage for 0.1C is 4.2, for 1C it is 4.1, for 2C it is 4 and for 4C it is 3.8. Discharge capacity is also different for different C-rates, discharge capacity for 0.1 C is 15.1, for 1C it is 14.9, for 2C it is 14.7, for 4C it is 12.8. So in this we can clearly observe that with the increase in C-rate discharge capacity is increasing. Let's observe this for other values of thickness. Further we will see how we will vary the thickness and the voltage vs discharge capacity will change

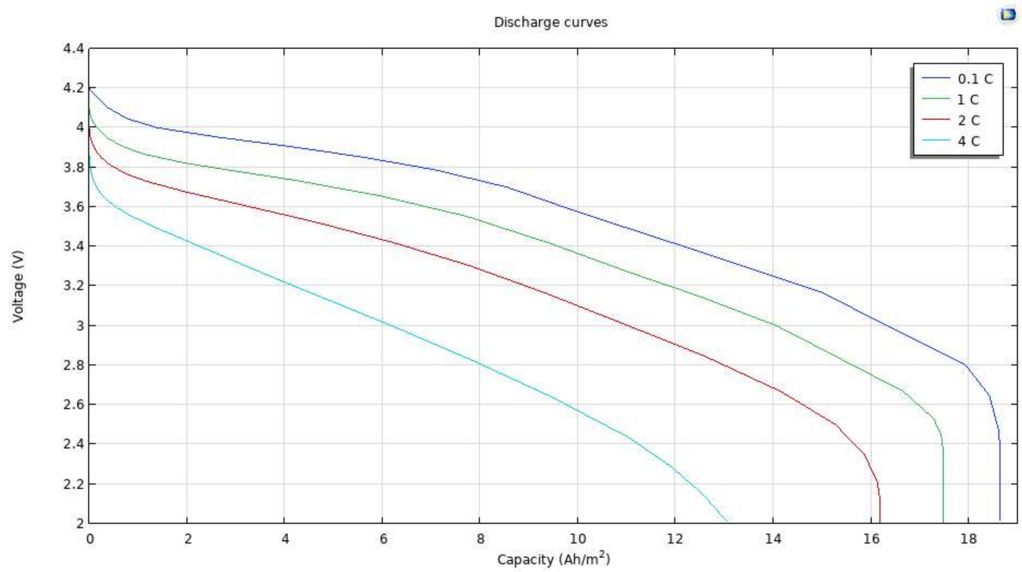

Figure 5.4 Electrode of thickness 125μ m

As we can see for cathode of thickness 125μ m voltage is different for different C-rates, voltage for 0.1C is 4.2, for 1C it is 4.1, for 2C it is 4 and for 4C it is 3.8. Discharge capacity is also different for different C-rates, discharge capacity for 0.1 C is 18.7, for 1C it is 17.6, for 2C it is 16.2, for 4C it is 13. So in this we can clearly observe that with the increase in C-rate discharge capacity is increasing. Let’s observe this for other values of thickness. Further we will see how we will vary the thickness and the voltage vs discharge capacity will change.

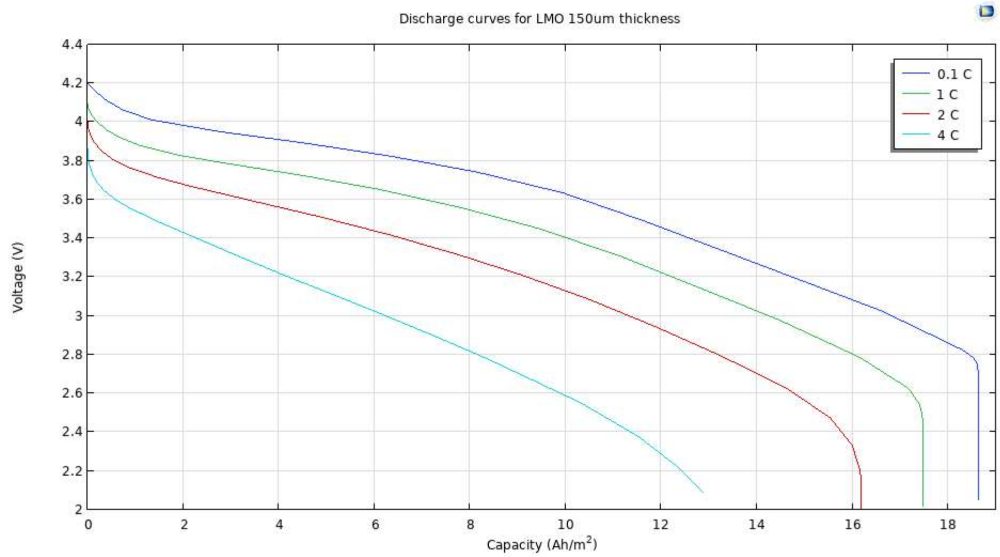

Figure 5.5 Electrode of thickness 150μ m

As we can see for cathode of thickness 150μ m voltage is different for different C-rates, voltage for 0.1C is 4.2, for 1C it is 4.1, for 2C it is 4 and for 4C it is 3.8. Discharge capacity is also different for different C-rates, discharge capacity for 0.1 C is 18.6, for 1C it is 17.7, for 2C it is 16.2, for 4C it is 13.2. So in this we can clearly observe that with the increase in C-rate discharge capacity is increasing. Let's observe this for other values of thickness. Further we will see how we will vary the thickness and the voltage vs discharge capacity will change.

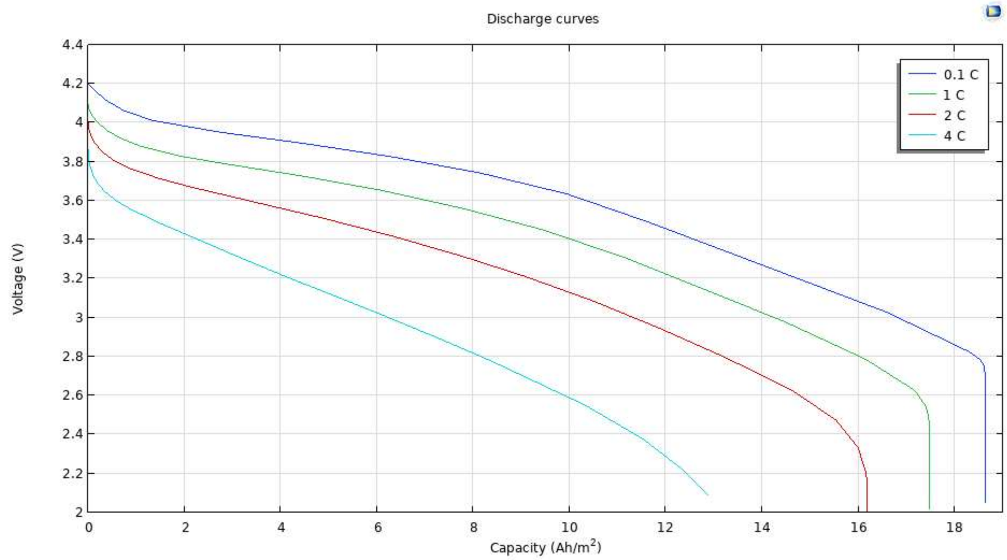

Figure 5.6 Electrode of thickness 175μ m

As we can see for cathode of thickness 175μ m voltage is different for different C-rates, voltage for 0.1C is 4.2, for 1C it is 4.1, for 2C it is 4 and for 4C it is 3.8. Discharge capacity is also different for different C-rates, discharge capacity for 0.1 C is 18.6, for 1C it is 16.7, for C it is 16.2, for 4C it is 13.2. So in this we can clearly observe that with the increase in C-rate discharge capacity is increasing. We have seen that with increase in thickness there is no much change in discharge capacities and voltages at different C-rates.

CHAPTER-6

CONCLUSION

When we increase the thickness of electrode we basically increase the path length which lithium ions need to cover before they reach the electrode which in turn affects many other characteristics like charges developed which arises due to polarization and the process in which bulk transfer of ions take place. We also observed that when we increased the thickness of positive electrode discharge capacity is increases but after a certain thickness it gets saturated which can be due to the sensitivity of thicker electrode towards discharge capacity. Due to increase in thickness of positive electrode we can see more lithium ions which are present between positive and negative electrode during the process of charging-discharging. We also got to know that for higher C-rates discharge capacity was low as compared to the lower C-rates. This can be due to the internal resistance which was produced due to the high temperature because for higher C-rates energy is high and due to which temperature rises.

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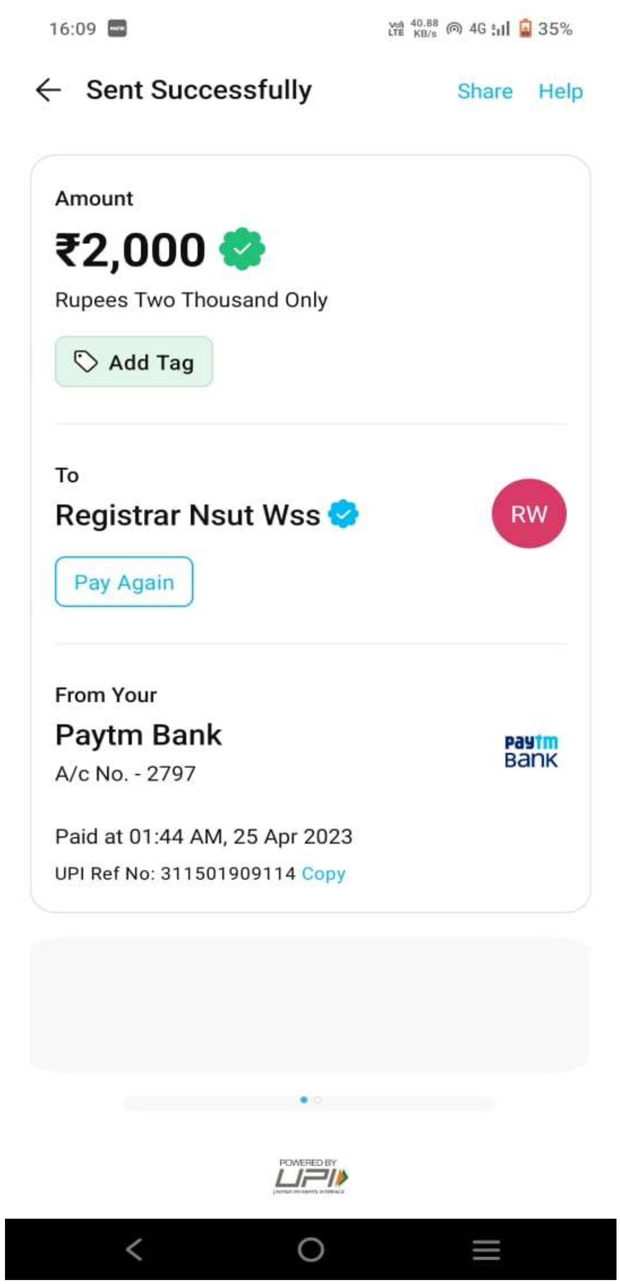
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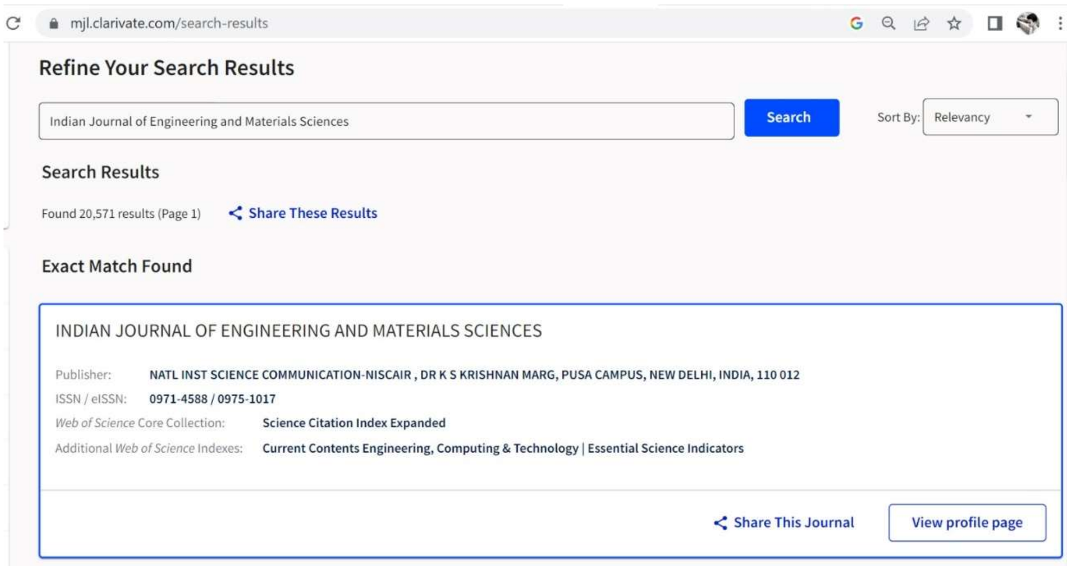
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