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Computational Modelling of Surface Modified Carbon Nanotube for Low Temperature Fuel Cell

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For the advancement in performance of a PEMFC (Polymer Electrolyte Membrane Fuel Cell) it is seen that computational modelling plays a key role. It is observed that the fuel cell catalyst layer gives many challenges from a modelling standpoint. It comprises of a complex, multiphase nanostructured porous material which is difficult to characterize. Carbon nanotubes (CNTs) are excellent support structures for the anode catalyst layer because of their electrical, mechanical and thermal properties, as well as their huge application potential. Among different functionalization methods, ion irradiation has proven to be an exceptionally effective method for modifying and adapting the properties of CNTs, especially Multi-Walled Carbon Nanotubes (MWCNTs), by creating defects and adjusting the structure in a controlled manner. As functionalization by the irradiation technique is still undergoing intense development, the combination of new and optimized materials with high electrocatalytic activity and optimization of the conditions for this method is expected to lead to a significant increase in performance, efficiency and cost-effectiveness. Computational modelling makes it possible to systematically simulate and optimize functionalization conditions, which would facilitate the preparation of a new electrocatalytic material. Moreover, modelling of CNT functionalization gives in-depth understanding of the structure and transformation of CNTs upon ion irradiation. This model can be used to predict the electrocatalytic activity of an electrode like a function of physical characteristics as intrinsic activity of catalyst. This work exhibits computational modelling of a modified catalyst layer for a PEM fuel cell system by using MATLAB and PYTHON as programming languages.

Keywords: Fuel cell, Surface modification, Carbon nanotube, Simulation.

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1. INTRODUCTION

Fuel cells are highly promising as a source of alternative energy and specifically PEMFC have attracted much attention recently as potential mobile power sources. It is well known that in an operating fuel cell the catalyst layer (CL) functions as a gateway for the transport of charged species that is electron and protons and also for the non-charged and gaseous species that is oxygen, hydrogen, water [1-3].

It is seen that the transport of charged species takes place in solid phase – protons in ionomer and electrons in carbon/Pt to be precise but for non-charged species and phase change of water takes place in the gas pores and ionomer phase. In the vicinity of catalyst (Where ionomer and carbon are present) electrochemical reaction happen. Product water from the cathodic reaction may exist in several phases simultaneously (gas, liquid, absorbed water in the ionomer, and ice under extreme conditions) depending on the thermodynamic state, which further depends on local heat transfer and mass transport. The usual method of fabrication of a Catalyst Layer by mixing ionomer and Carbon Platinum particles gives a porous medium full of interfaces. The catalyst layer has presented several challenges for modelling, such as (1) coupled transport and reactions, (2) wide range of length scale, and (3) multiphase flow. The conventional method of fabrication of a CL by mixing ionomer and C/Pt particles yields a porous medium full of interfaces. Surface modified carbon nanotube supported Pt based catalysts are emerging as a promising catalyst.

Therefore, modelling the surface modified catalyst layer is very important for the better understanding of the electrochemical activity of the catalysts [4-7]. Multi walled Carbon nanotubes have remarkable electrical, mechanical properties and high aspect ratio. Their genuine one-dimensional structure is quite well-suited for studying the effect of disorder on the properties of low dimensional systems. Ion irradiation is a very good tool for adjusting the defects and structures in carbon nanotubes and this technique involves the bombardment of foreign ions towards the nanotube lattice, thereby creating defects in a controlled fashion. This defect formation is responsible for the creation of single and double vacancies. The main reason behind this defect formation is the transfer of kinetic energy by the bombarded ions to the nanotube lattice atoms. The extent of this defect formation is well understood by a parameter known as the displacement per atom (dpa) which is a very useful tool for understanding the extent of surface modification of a carbon nanotube via ion irradiation. This ion irradiation technique is particularly significant as here the defects are created in a controlled fashion [8, 9]. Ion irradiation leads to some defects in MWCNT, alters the CNT composition due to ion incorporation. The irradiation conditions namely dose, ion mass, energy, ion bonding, effect of temperature and substrate are also important parameters to be

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considered. The ion irradiation process affects the electrical, mechanical and field emission properties of carbon nanotube. So, this study aims at the modelling of ion irradiation conditions to get the CNT surface modified best electro catalysts.

2. TOOLS

For the modelling of the irradiation technique on CNT, MATLAB (Version 21) and PYTHON (Version 3.9.6) were used.

3. RESULTS AND DISCUSSION

In Fig. 1, we observe the variation of energy of incident ions with the density of states. It is observed that as the density of states increases more energy of incident ions is required for causing the displacement per atom. The plot is linear ideally. But we observe some deviations from linearity depending on the modelling of carbon nanotube along a certain axis and also with increase of diameter. Here outer diameter of our chemically functionalized carbon nanotube is 30-50 nm. The length of nanotube used is 10-30 micrometres. The *M* value is 1 and the n value is 0. The electrical conductivity is similar to that of a metal or a semiconductor. The density of states increases with the outer diameter of the carbon nanotubes.

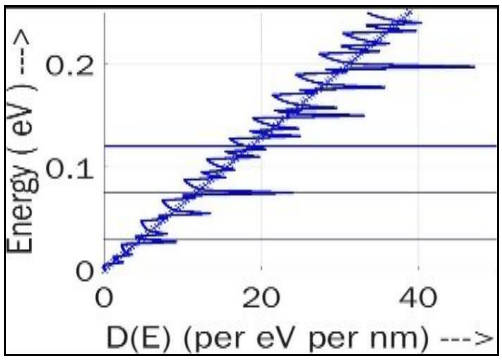

Fig. 1 – The variation of energy of incident ions with the density of states

In Fig. 2, the solid curve represents the entire band structure. The dashed curve represents the dispersion nature obtained for one band effective mass. There are two dashed curves in the figure. For one it is observed that energy of incident ions is increasing with increase of fraction value. For the other it is observed that the energy of incident ions is decreasing with increase of fraction value. In this case the aim has been to create an optimized condition where the effect of ion irradiation on carbon nanotube for surface modification can be better understood. Here the maximum value is the total gap between the valence band and the conduction band. We are interested in taking a fraction of the maximum value because the fractional situation enables us to control vacancy formation in a facile manner and gives us a better understanding of the change in electrical, mechanical and solubility properties due to ion irradiation. Taking the maximum value is not beneficial as the maximum value corresponds to the situation where the vacancy formation is random and cannot be controlled.

In Fig. 3, the variation of energy of incident ions with the density of states per unit area is observed. AS the density of states increases, the energy required to cause the displacement per atom also increases progressively. The transition from 2-dimensional to 3-dimensional model elucidates the transition towards a macroscopic picture with increase of density of states. Here the area involved corresponds to the cross-sectional area of the circle present inside the nanotube and this helps in the better understanding of the transition from 2-dimensional to 3-dimensional picture.

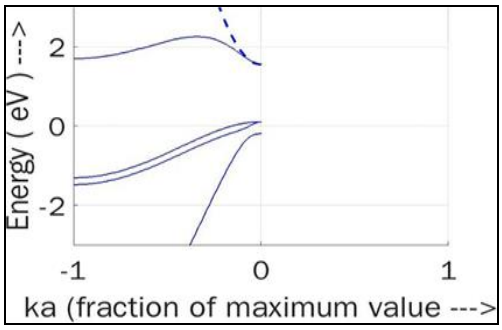

Fig. 2 – The energy of incident ions with the K_a

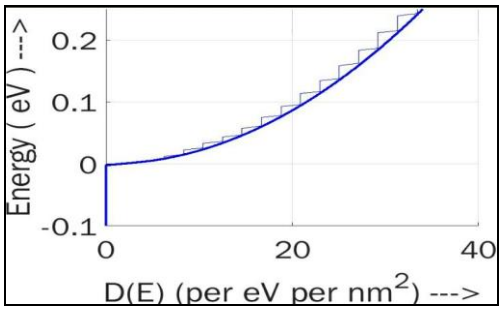

Fig. 3 – The irradiation energy with the density of states per unit area

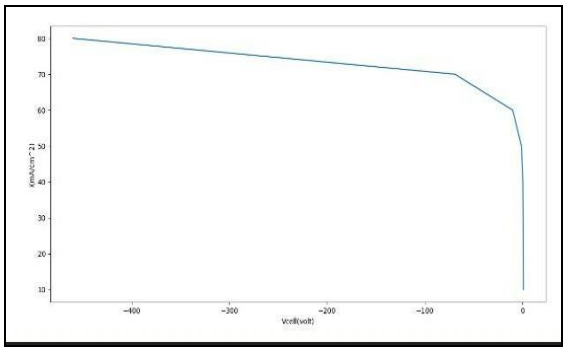

Fig. 4 – The loss of voltage with increase of current density

The python plot (in Fig. 4) depicts the loss of voltage with increase of current density. It is observed that the ohmic loss exhibits a steady but non-linear increase with increase of current density. This clearly elucidates the resistance occurring due to the ohmic nature of the electrical conduction and the voltage drop due to the resistance arising out of this ohmic nature. We know that as per Ohm's Law: $V/I = R$. In this case this R is responsible for the Ohmic loss. These losses arise due to the hindrance faced by the electrons while travelling through the electrolyte or membrane and represents

the overall slowing down of the movement of electrons due to the electrolyte ions present in the environment.

In Fig. 5, an energy dispersion relation explains the condition of the 4 lowest valence band sub bands and a beautiful mathematical step function is observed. The x-axis represents the energy of band whereas the y-axis represents the kinetic energy of the irradiated ions (difference between the total energy and the work function of the ions).

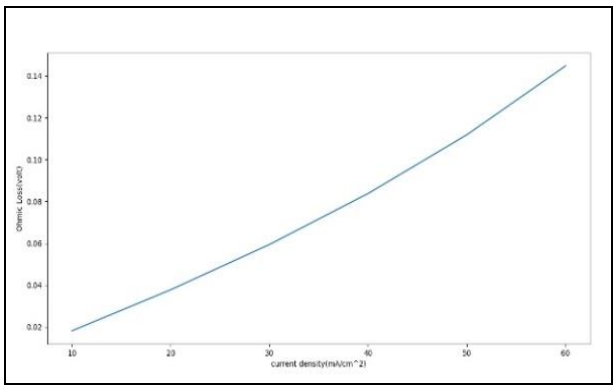

Fig. 5 – An energy dispersion relation

Fig. 6 represents the variation of current density with increase of voltage for a PEM fuel cell. This clearly shows that at low potentials current density is high and after a certain point the current density drops abruptly. The area under this curve gives the magnitude of the power density produced. This is because $P = I \cdot V$. Here the current density falls abruptly to 0 as with the completion of transfer of ions, the scope of potential difference generation in the closed circuit is eliminated and as a result after a certain time both voltage and current reduce to 0.

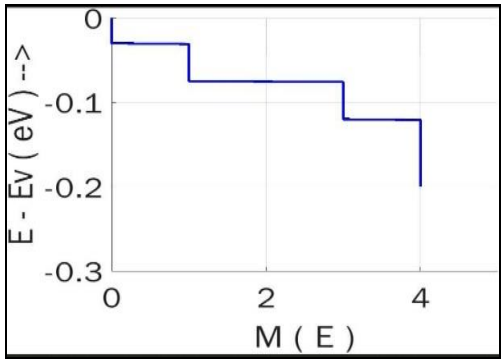

Fig. 6 – The variation of current density with increase of voltage

4. CONCLUSIONS

Carbon nanotube modification is very useful for the development of a PEM fuel cell. Ion irradiation is a very important technique for MWCNT modification. PYTHON/MATLAB programming language can be used for computational modification and study of fuel cell properties.

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Обчислювальне моделювання поверхнево-модифікованої вуглецевої нанотрубки для низькотемпературного паливного елементу

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Обчислювальне моделювання відіграє ключову роль для підвищення продуктивності PEMFC (Polymer Electrolyte Membrane Fuel Cell, паливний елемент з полімерно-електролітною мембраною). Помічено, що шар каталізатора паливного елементу створює багато проблем з точки зору моделювання. Він складається зі складного багатофазного наноструктурованого пористого матеріалу, який важко охарактеризувати. Вуглецеві нанотрубки (CNTs) є чудовою опорною структурою для шару анодного каталізатора завдяки своїм електричним, механічним та термічним властивостям, а також величез-

ному потенціалу застосувань. Серед різних методів функціоналізації іонне опромінення виявилося виключно ефективним методом для модифікації та адаптації властивостей CNTs, особливо багатостінних вуглецевих нанотрубок (MWCNTs), шляхом створення дефектів і контрольованого регулювання структури. Оскільки функціоналізація методом опромінення все ще знаходиться на стадії інтенсивного розвитку, поєднання нових та оптимізованих матеріалів з високою електрокаталітичною активністю та оптимізація умов для цього методу, як очікується, призведе до значного підвищення продуктивності, ефективності та економічності. Обчислювальне моделювання дає змогу систематично моделювати й оптимізувати умови функціоналізації, що полегшило б отримання нового електрокаталітичного матеріалу. Крім того, моделювання функціоналізації CNTs дає глибоке розуміння структури та трансформації CNTs під час іонного опромінення. Цю модель можна використовувати для прогнозування електрокаталітичної активності електрода як функції фізичних характеристик, таких як внутрішня активність каталізатора. Дана робота демонструє обчислювальне моделювання модифікованого шару каталізатора для системи паливних елементів PEM з використанням мов програмування MATLAB і PYTHON.

Ключові слова: Паливний елемент, Модифікація поверхні, Вуглецева нанотрубка, Моделювання.