Abstract
This thesis aims at contributing towards development in pH sensing by proposing a novel device structure of Ion Sensitive Field Effect Transistor (ISFET) and a detailed physico chemical model for its simulation to predict the device characteristics particularly at nano dimension.

Intracellular pH is an important cell function modulator. The activity of proteins depends on pH. Delivery, absorption and effectiveness of drugs can be altered by changing the pH of the local environment. If pH falls below 6.8 or rises above 7.8, the person may die. In certain medical and biotechnological research it becomes necessary to extract signals from within a cell. Intracellular pH difference across the mitochondrial membrane drives the electron transport chain which converts electron energy in to phosphate bonds. For such purpose, sensor capable of extracting information from a single cell is highly essential. In order to achieve clear understanding of what is happening inside a single cell, sensor must meet the physical dimension, detection limit and sensitivity precisely.

The concept of Ion Sensitive Field Effect Transistor was first proposed by Prof. Piet Bergveld, in the year 1970. The basic device is sensitive to $H^+$ ions and hence it can give a measure of pH of the solution. Field Effect Transistor has shown its suitability as a bioelectronic device for biosensor and has undergone several changes and transitions since its inception in the year 1970. Since then a good number of papers have been published in different journals/conferences. The research work seen so far shows flow of ISFET research mainly in two directions: - one of which shows some experimental results with new samples, new materials to establish the potential of the device in a new direction of application.
In the other direction of research it shows the development of a model -may be a physico-chemical or may be a model based on SPICE (Simulation Program with Integrated Circuit Emphasis) for different sensing materials. The objective of such work is to find out a new material that can be used to make devices with enhanced sensitivity.

A unique feature of all the papers is that, the work is based on the conventional planer device. It has also been observed that no research group or individual has so far worked on a new device geometry or shape for enhancing sensitivity of the ISFET. The potentiometric sensitivity has very weak dependence on device geometry, but the amperometric sensitivity which is highly dependent on device transconductance is in turn dependent on the device geometry. By using appropriate material for gate insulator and/or sensing surface of ISFET, the device sensitivity can be enhanced to a particular level. In case of an in vivo sensor it may not always be possible to use the material with highest sensitivity, when the question of biocompatibility arises. In this situation some other methods for sensitivity enhancement will be required, such as new device geometry. In addition ISFET in its planner form when scaled down to deca nanometer dimension comes up with numerous small dimension effects. The Gate All Around MOSFET Structure is very successful against most of these parasitic effects and when these structures are implemented for the ISFET, the sensor amperometric sensitivity shows much higher value. Among all the gate all-around structure, the cylindrical structure is the best because of absence of corner effect. Corner effect gives rise to non uniform gate overdrive and consequently current density also becomes non uniform. This problem is not encountered in Cylindrical Structure.
The main purpose of this work is to develop a Physico chemical model of Cylindrical ISFET of nano dimension. Nano dimension is chosen because; the intended application of this device is for single cell monitoring. Here in this work a complete model of this device has been developed considering the entire major small dimension effects including the quantum mechanical (QM) effects leading to threshold shift. While the initial simulation results (in the sub micron range) have been compared with the data available in literature to evaluate consistency of the model, subsequent results (in the nanometer range that includes QM effect) provides prediction about the device response. This work also gives a rule for reference electrode placement. This finally determines the overall system dimension which depends upon the Debye length corresponding to the highest value of pH to be measured.

The first part of the thesis discusses basics of ISFET, fundamentals of oxide/electrolyte interface of the site binding model and physico chemical modeling of the device. In this part a generalized model for the planer ISFET are discussed based on the site binding model for silicon dioxide as sensing material. Silicon dioxide, when used as pH sensing surface posses only one type of surface site.

Attempts have been made in a very modest way to contribute the following in the present thesis:-

1. First, a novel ISFET structure has been introduced based on the surrounding gate MOSFET which is available in literature. A physico chemical model for the same has been developed in this work. Here the semiconductor charge has been considered as two distinct layers – inversion layer and depletion layer and the simulation results show the followings.
Above threshold condition the inversion charge depends on pH and the depletion charge remains fixed, below threshold, the depletion charge shows its dependence on pH.

The Diffuse layer at the electrolyte insulator interface surrounding the cylindrical device is influenced by cylindrical geometry. This influence is also modeled and analyzed. The device model is simulated in MATLAB and its behavior is analyzed for various pH values. The results show sharper fall in diffuse layer potential compared to the planer geometry. Deviation of device potentiometric sensitivity as a function of reference electrode position relative to the OHP (Outer Helmholtz Plane) has also been analyzed.

The results obtained from simulation leads to the conclusion that there is a definite correlation between the distance from the OHP to the reference electrode and the Debye length of the electrolyte at that particular value of pH. A distance of 3 Debye lengths can give results having one to one relationship between electrolyte oxide interface potential and pH i.e. one value of electrolyte oxide interface potential corresponds only to one value of pH. If the reference electrode is placed at a distance smaller than the Debye length from the OHP in a particular range of pH one value of electrolyte oxide interface potential will correspond to two values of pH.

2. A humble attempt has been made to develop the cylindrical ISFET at nano dimension. In this part of work study was carried out giving emphasis on the following factors:

a) The conduction band edge shift at nano dimension has been considered by solving the Schrödinger Wave Equation in cylindrical coordinate.
b) The increase in effective oxide thickness (EOT) that occurs due to shifting of inversion layer centroid away from the insulator semiconductor interface has also been considered.

The study that was carried out on the developed model by considering the above two factors reveals an increased threshold voltage resulting lower drain current at a particular reference electrode voltage and at a particular value of pH.

3. Further, the effect of insulator thickness on the sensitivity of the device was also studied. When the insulator thickness is reduced to nano level, the number of buried (slow responding) sites reduces in number, while the number of surface (Fast responding) sites remains the same. At insulator thickness equal or less than 3 nm, there is no buried site present, consequently when this effect is incorporated in the model developed in (2) little lesser potentiometric sensitivity obtained, but the output settles faster.

While including the nano dimension effects as discussed in (2) it is observed that the drain current and potentiometric sensitivity of the device decreases, and consequently the amperometric sensitivity also decrease. Even though these three factors pulling the device current and the amperometric sensitivity down at nano dimension, the results are much better while compared with the planer device at similar dimension, which is due to better device transconductance arising out of the device geometry.

When the rule for reference electrode placement is implemented to the cylindrical device, it is observed that, to obtain the same amount of
potentiometric sensitivity, the reference electrode in a cylindrical ISFET can be placed at a smaller distance from the OHP as compared to that in a planer device.

It can therefore be conclude that cylindrical device provides a pH measuring system with smaller dimension with higher amperometric sensitivity as compared to the planer device.

As a future extension of this work, the temperature variation of human body may also be considered in the model because, temperature change in human body under diseased condition may be sufficient to cause drift in the ISFET response in vivo.