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Observation of Modified Poisson Boltzmann and Poisson Boltzmann Models on Silicon Nanowire Field Effect Transistor in Electrolyte Environments for Sensing Applications

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Abstract: Recognizing the electric double layer properties in nanowire FET is important not only in electrochemistry but also in a wide variety of areas including biosensors, colloid science, membrane biology, and separation phenomena. The implementation of modified Poisson Boltzmann model on one dimensional nanostructures in electrolyte environments is very interesting field. In this work, the modified Poisson Boltzmann and Poisson Boltzmann model implemented in Silicon Nanowire Field effect transistor in common electrolytes environments for noticing the characteristics both the models. The ionic distributions profile and the electric double layer potential drop profiles of the MPB and PB models have compared and the results exhibited. The MPB model of NaCl, CsCl electrolyte environments and the PB model electrolytes environments of electric double layer potential drop with various concentration results compared. The results show the MPB model provides higher resolution than PB model for a given surface charges. while designing of the sensors the MPB model results should be considered at specified parameters.

Keywords: Biosensor, Comparison of MPB and PB, Electrical double layer Analysis, Silicon Nanowire FET

1. INTRODUCTION

Many of the theoretical work was developed for analyzing double layer properties of inner and diffuse parts since 1970s by using simple electrodes. So far, Gouy Chapman (GC) and related to theories only used by most experimentalists [1,2] Because the other theoretical works involved complicated mathematical equations, which often due to the absence of analytical solutions.

Bikerman, showed the change of the distribution function from the Boltzmann functions by taking into finite volume of ions [3]. The finite size ions may play an important role in a concentrated solution. After that, Borukhov et al [4,5], developed the simple modified poison Boltzmann model which includes the steric effects in electrolytes environment and it has been reinvented many times by kilic Bazant et al.[6,7] and Kornshev [8].The importance of Modified Poisson Boltzmann equation in electrical double layer is explained Lou et al [9] and Ping et al. [10]

The significant device applications of One dimensional nanostructure of nanowire were clearly described by Thomas Mikolajick [11]. The sensitivity of Nanowire FET and the electrochemical detection of the nanowire FET discussed in detail [12,13]. The well-developed Schottky barrier nanowire FET model in liquid environments shown by Nozaki et al [14]. In our previous work we have shown the finite size ions effects in various electrolytes environments by implementing the modified Poisson Boltzmann model on nanowire field effect transistor for the designing of sensor applications [15].

In this work, we have applied the exact analytic expression of the modified Poisson Boltzmann and the Poisson Boltzmann equation on the nanowire FET for noticing the characteristics between the counterion and coion distributions profiles as well as electric double layer potential drop appearances at negative charge densities for the given 1:1 electrolytes concentrations.

2. MPB AND PB MODEL DISCUSSION

The modern Modified Poisson Boltzmann (MPB) theory is commonly used in the electrolyte environments. The modified part of the Boltzmann distribution in the MPB equation of co-ions is given by,

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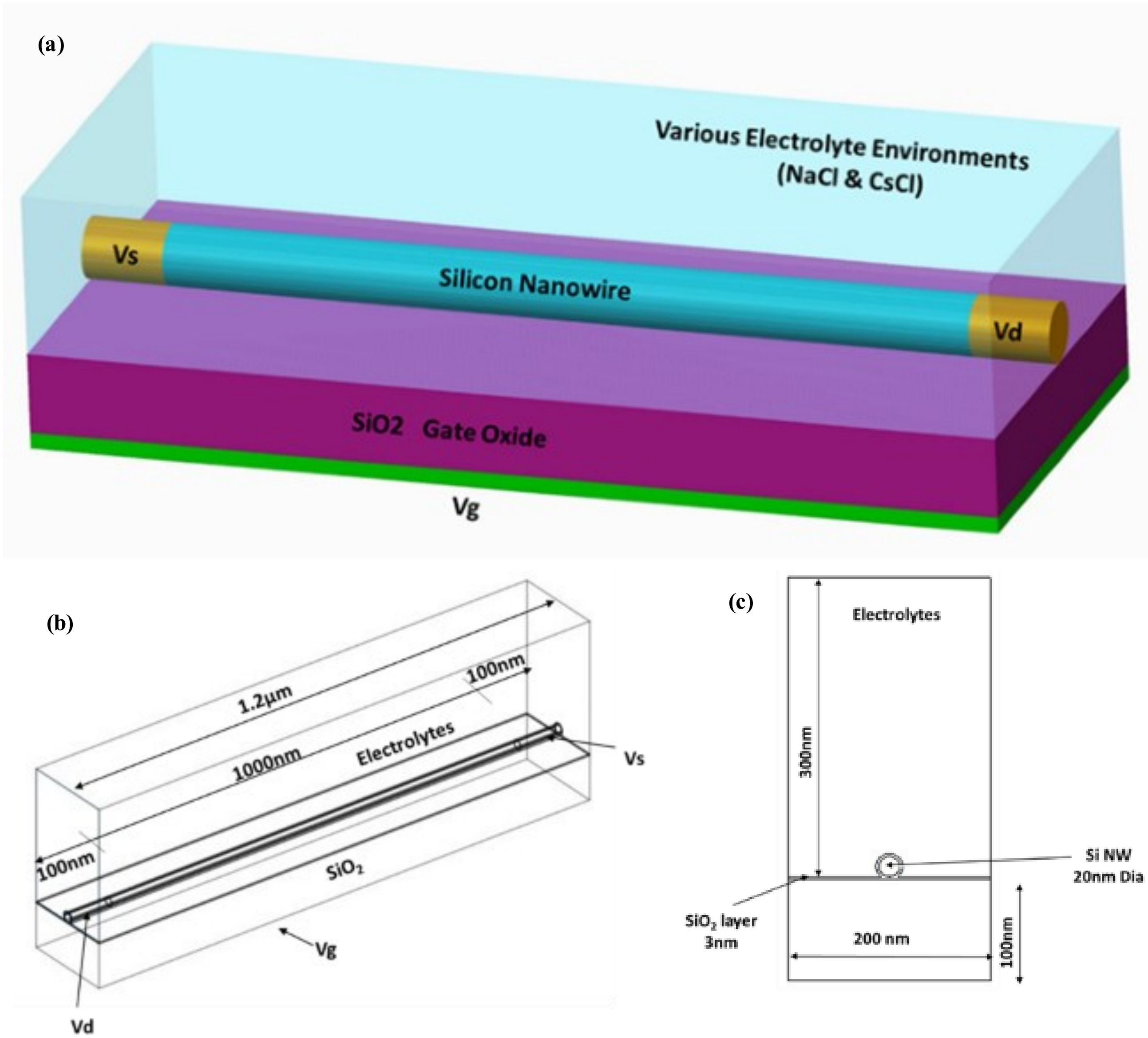

Figure 1. (a) 3D view of Nanowire FET model in electrolyte environments. (b) 3d view of schematic device model (c) 2d cross section area view of device model.

$$c_i^-(r) = \frac{c_i^\infty \exp(-\frac{z_i e\psi(r)}{kT})}{1+2v\sinh^2(\frac{z_i e\psi(r)}{2kT})} \tag{1}$$

For counterions,

$$c_i^+(r) = \frac{c_i^\infty \exp(\frac{z_i e\psi(r)}{kT})}{1+2v\sinh^2(\frac{z_i e\psi(r)}{2kT})} \tag{2}$$

In Equations (1) and (2), $v = (z+1)a^3c^\infty$ is the total volume fraction of the positive and negative ions (called the packing parameter) and a is the effective ion size. We have taken a binary symmetric electrolyte and assume that the surface of the nanowire FET has a negative charge. Thus, we have $z=|z+|=|z-|$ and $c^\infty=c_+^\infty=c_-^\infty$, so the Borukhov et al., MPB equation can be rewritten as,

$$-\varepsilon\nabla^2\psi(r) = -zec^\infty \frac{2\sinh\left(\frac{z_i e\psi(r)}{2kT}\right)}{1+2v\sinh^2\left(\frac{z_i e\psi(r)}{2kT}\right)} \tag{3}$$

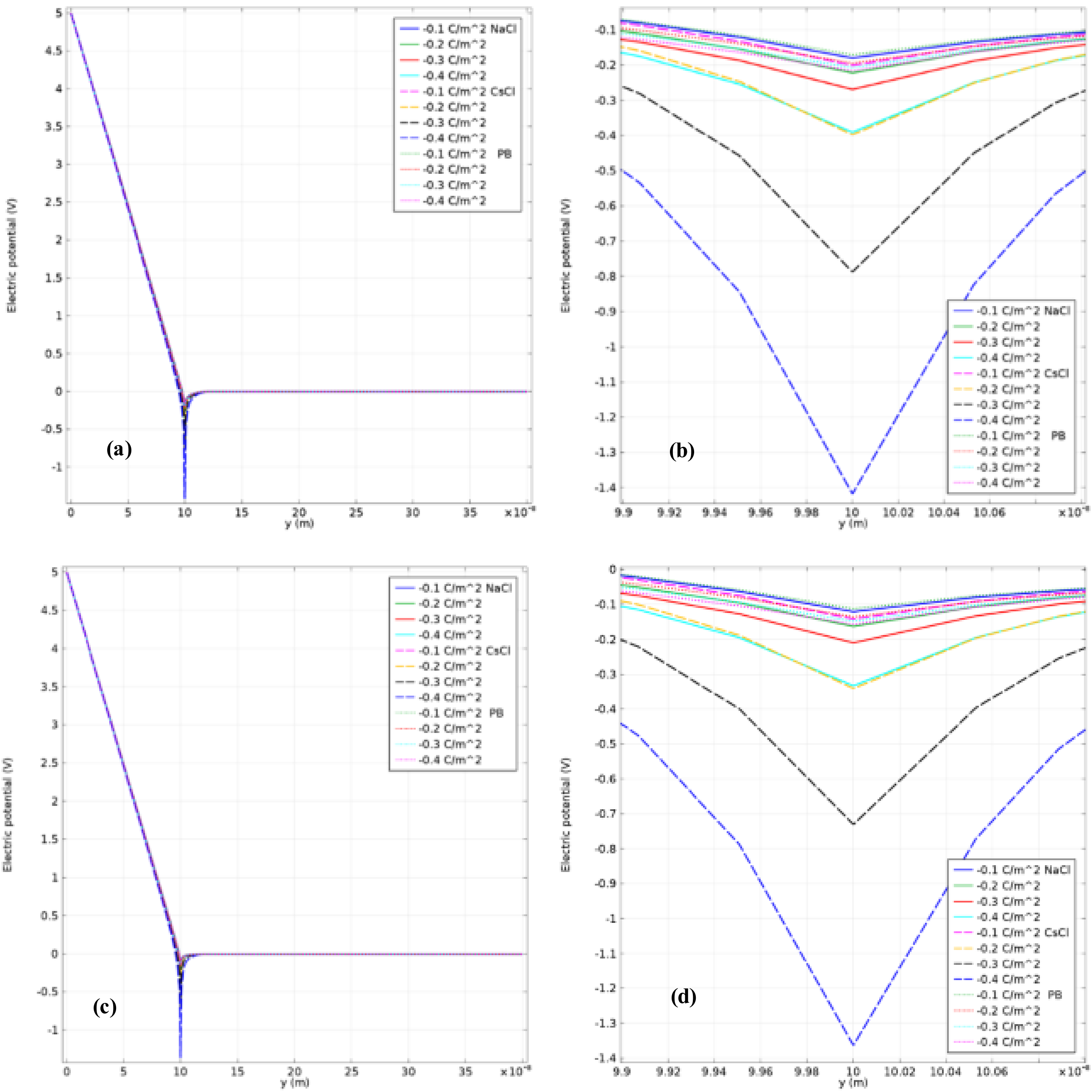

Figure 3. Electric double layer comparison of PB and MPB model on nanowire FET in 0.1M (a) and 1M (c) concentration corresponding enlarged view (b, d). Solid line shows NaCl, dashed line shows CsCl and dotted lines shows PB values

In equation (3), where $\psi(r)$ is the electric potential forces that act on each ion, c_i^∞ is the bulk concentration of the ion "i", z_i is the valence number of ion "i", e is the proton charge (1.6×10^{-19} C), T is the temperature (°K) and k is the Boltzmann constant (1.38×10^{-23} J/°K). The molar ionic concentrations M_i expressed as $M_i=c_i^\infty 10^{-3}/N_A$. Where N_A is the Avogadro constant (6.022×10^{23}). $\varepsilon=\varepsilon_0\varepsilon_r$, ε_r is the relative permittivity of the solution and ε_0 is the dielectric constant of the vacuum. The relative permittivity for water, Si, and SiO_2 are used in 80, 12.1, and 4.2, respectively. By including the effective ion size in modified Poisson Boltzmann equation, which includes the steric effects and makes clear resolution in results for designing the sensor. By making ion size is equal to zero these equations reduce to standard Poisson Boltzmann equation and it make it is point like charges without the steric effects.

3. DEVICE MODEL

In order to analyze electrical double layer potential and the ionic distribution characteristics for various ionic concentrations with

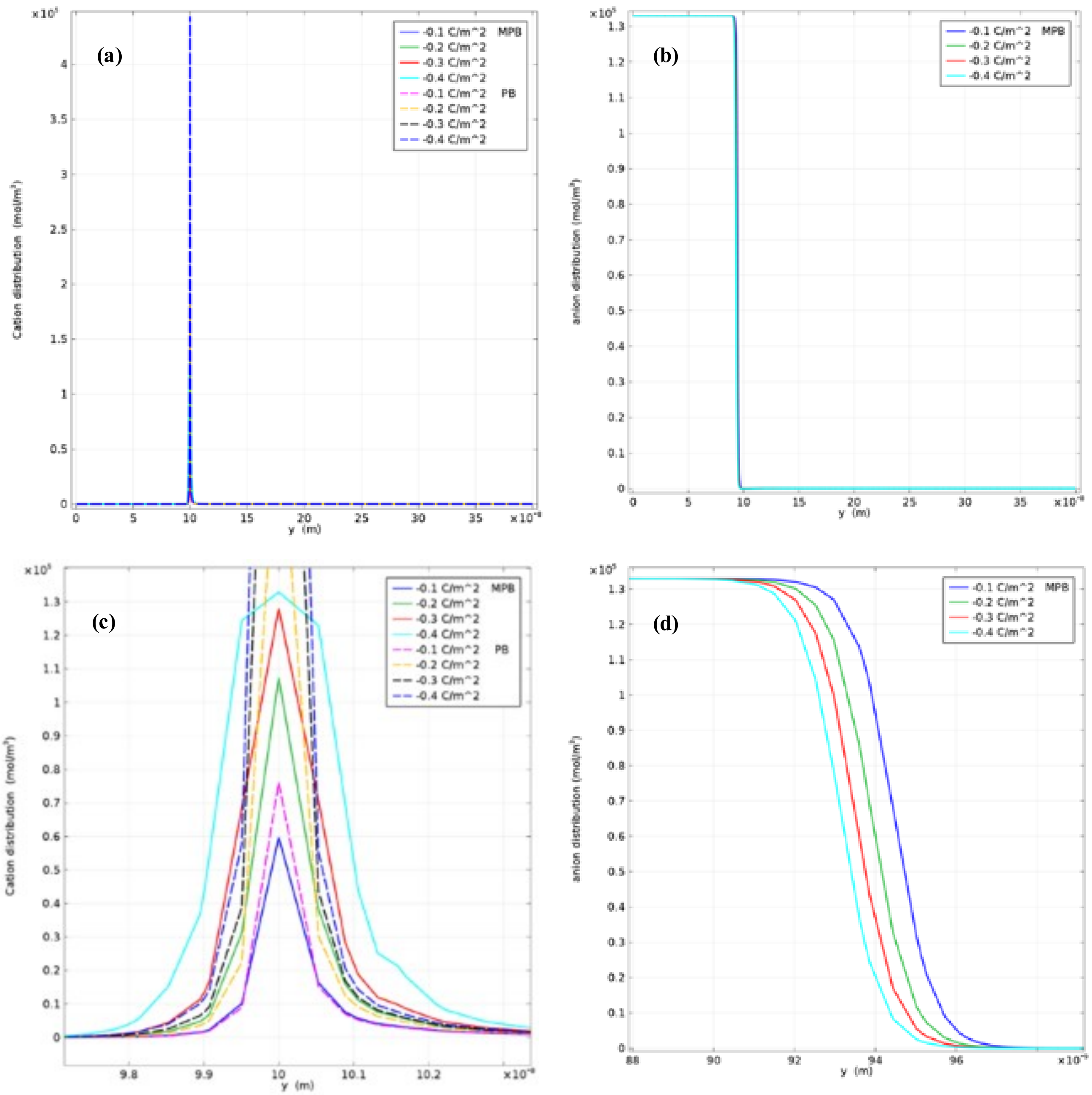

Figure 2. Ionic profile results between MPB and PB model implemented on nanowire FET. (a) Cation (b) anion distributions in NaCl solution 0.1M concentration and (c, d) corresponding magnified view

finite volume ions, we subjected our Silicon nanowire Schottky barrier FET 3 D device design with the implementation of Poisson Boltzmann and modified Poisson Boltzmann equation model in liquid environment. The 3D and 2D device geometry as shown in figure 1 (a, b & c). The channel length of the semiconducting Silicon nanowire was 1000nm and the diameter was 20 nm. the length of the source and drain contacts were 100nm.

3nm SiO2 native oxide layer was covered entire nanowire surface. The top of the layer was surrounded the aqueous environment providing electrolyte concentration. The thickness of the gate oxide insulator and the liquid phase are set to 100 nm and 300 nm, respectively. After modeling and the setting the parameters the device geometry, the PB and MPB equation is solved numerically using Finite element analysis software. In the solid-liquid interface, the surface charge density is applied in between the Si nanowire and the electrolyte concentration. Gate, source, and drain, electric potentials are applied to the respective contacts. For all calculations, a gate voltage Vg of 5V and a drain voltage Vd of 0.5V is used.

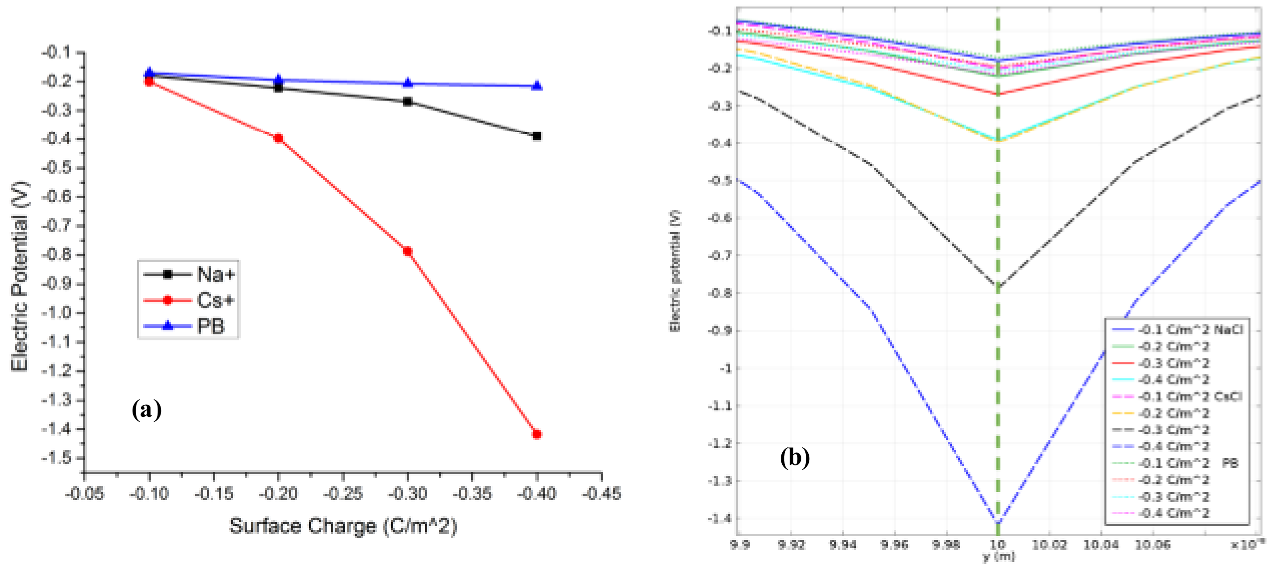

Figure 4. (a) Electric potential Comparisons of Na+, Cs+ ions in MPB model and PB model (in the position of Dashed green line, (b) with change of surface charges from -0.1 to 0.4 C/m^2.

4. RESULTS AND DISCUSSIONS

4.1. Comparisons of PB and MPB model ions distribution profile on nanowire FET

For comparing the MPB and PB equation models on nanowire FET, we have chosen lower ion radius NaCl and higher ion radius of CsCl electrolyte solutions. We have taken NaCl, the effective ion size, *a*, of Na is 2.32 × 10–10 m and in CsCl *a* of Cs is 3.2 × 10–10 m and the concentration have taken 0.1M and 1M. Here, we have considered the surface charge density in the range between –0.1to –0.4 C/m^2.

Figure 2. shows the comparisons between ionic distributions profile with the nanowire positions. Fig.2 (a & b) shows the cation and anion distributions of the 0.1M concentration of NaCl electrolytes used in MPB equation and the PB equation. From the magnified view of the figure 2(c & d), It is clearly seen the PB equation overestimates the cation distributions and in anion distribution, it produces indefinite results for the given surface charges. The ionic size effect plays important role when the negative charge density is higher than -0.1C/m^2 surface charges. From the results we can conclude the MPB equation produces the sensible results and the PB equation produces unthinkable results for the given surface charges.

4.2. Electric Double Layer Comparisons of PB and MPB model on nanowire FET

The figure 3. (a & c) shows the electric double layer potential profiles in various concentration of different electrolytes with MPB and PB equation models and fig. (b & d) shows the equivalent magnified view. In PB equation we could not find any difference in Na+ ions and Cs+ ions due to that, it considers ions as point like charges. The MPB model provides clear results for the Na+ ions profiles and Cs+ ions profile in double layer characteristics. In electric double layer characteristics always the PB equation underestimates the value. By taking account on this, we could design our sensing element properly by using the MPB equation. The ionic size effect becomes more important when the negative surface charge is larger than -0.1C/m^2.when the surface charge of nanowire FET is higher than -0.1 C/m^2 the potential drop of CsCl solution is higher than NaCl solution.

4.3. Electric Double Layer potential differences with the surface charge Comparisons

The figure 4.b shows the difference between Na+, Cs+ ions electrical potential drop and PB model potential drop at the position of dashed green line in fig 4.a. The potential drop of small ion Na+ is smaller than the larger ion of Cs+ for a given surface charge and concentration in nanowire FET. From the figure we can observe the PB equation produces the common results for the both the ionic solution since it is considered as point like charges and MPB equation produces clear results for the different ion sizes. The calculation performed here only the difference in NaCl and CsCl ion size. From the study we can conclude The MPB equation potential drop produces the clear results and PB equation deviates the original results since it does not consider the steric effects.

5. CONCLUSION

In this work, we have compared the PB model and the MPB model on the nanowire FET device in electrolyte environments. In the cation profile, the MPB shows the reasonable results compared with the PB model and in the anion profile the MPB shows the actual results but the PB equation shows the indeterminate. When compared into electric double layer characteristics, The Na+ and Cs+ ions shows the clear results while the PB model shows the underestimate values which is not suitable for sensor designing purpose at higher surface charge and concentration. The CsCl ions have higher potential drop due to the ion size is high than NaCl solution. But the PB model shows the insignificant values which is not acceptable for sensor design at particular specifications.

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