

## Modeling a Micro Tubule as a Diode

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### Abstract

All biological molecules and cell organelles are chemo mechanically controlled systems known to every biologist. The control signals governing them are electrical. The influence of an electric field in them makes a disturbance such that they behave as an electronic distributed network. It is an interdisciplinary art to activate them and work as an electronic device. Modeling the biological molecules as per the devices is by understanding their stability and work functions. Here a micro tubule (MT) molecule is modeled to function as a diode in electronic parameters, there by not disturbing its biological function. The MT is similar to its other cytoskeleton filament. In its two dimers alpha and beta, in the tunneling effect of the ions, can establish the diode characteristics in its conductivity of electric ionic current.

**Keywords:** Microtubule; Ionic current; Tunneling effect; Nanobiodevice

### Introduction

MT is one of the cytoskeletal filaments whose dimensions are in the range of nanometers. They contain two blocks known as (alpha) and (beta) dimers. They transfer the biopotential in the form of ionic currents which traverse in them by tunneling effect from one dimer to the other. To be more specific, the arrangement of the MT in the biological system forms a series of quantum wells arranged in order to transfer the biopotential signal to the neural network. In the dimers, the tunneling of the ions satisfies the Shockley diode's statistics. It could be modeled to work as a diode in a human body. It would also contribute more to the nanobioelectronics research work.

### Microtubule

Nanosized dimers of MT's constitute the conductivity channel for the electronic signals to the cytoskeleton for an action to be performed. The potential ranges are in the micro and the nano volt. The K<sup>+</sup>, Na<sup>+</sup> and Ca<sup>2+</sup> ions conduct the current in this channel. The MT is a part of the cytoskeletal neural network which transfers the biopotential into the ion channel to pass through them. They make the ionic circuit contact with the other external molecules through the terminal links. A MT molecule is made up of two lobes also called as dimers. The smaller lobe is called the alpha dimer and the bigger lobe is called as the beta dimer. Both of these lobes are interconnected molecules. The length of a MT is around eight nm. Its width and height are even lesser than its length. Arrangement of the MT molecules in a cytoskeleton network is known as a tubulin network arrangement. This is illustrated with a section of a MT in a tubulin network [figure 1](#).

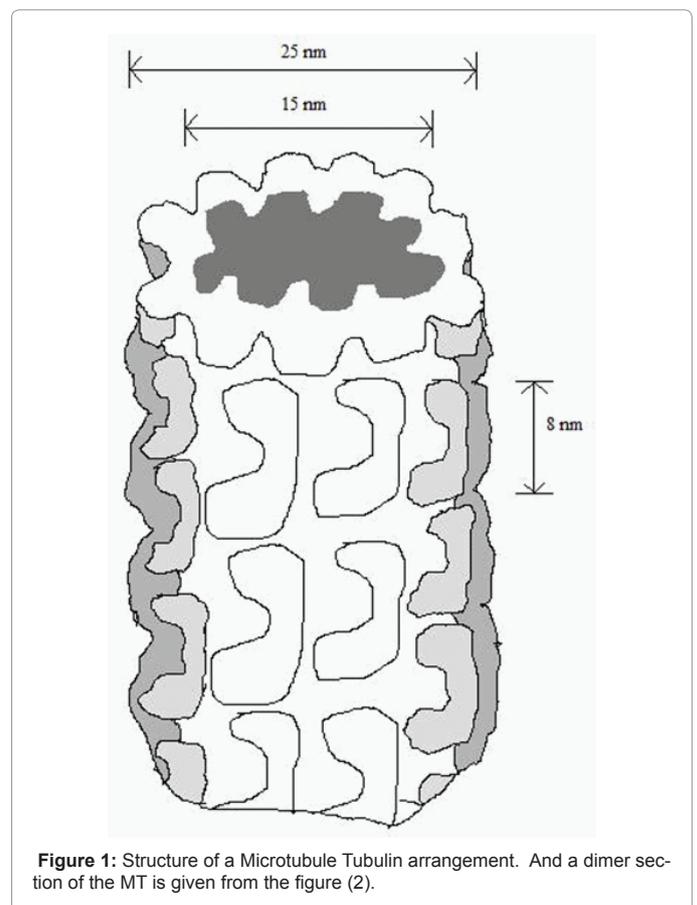
### General diode function

The general diode function of any semiconductor diode is to follow the Shockley charge transfer equation in a semiconductor, given by equation [1]. Voltage-Current characteristic of the proposed diode model is given in [figure 3](#). The diffusion of the charge carriers causes conduction to take place in the diode. An ideal diode is a unidirectional device that restricts the other reverse bias pair conduction theoretically.

$$I = I_s \{ \exp ( VD/nVT ) - 1 \}$$

equation 1. Shockley diode equation.

But in practical cases there is a leakage current flow in the diode when it is reverse biased. The same phenomenon when occurring in any other material other than a semiconductor is a very fascinating fact. The more the reverse bias extends the break down working of the device



occurs. Likewise, when it takes place in any biological molecule it would contribute to a nanobioelectronic device. The name nanobioelectronics has been mentioned because most of the biological molecules are of the nano dimension.

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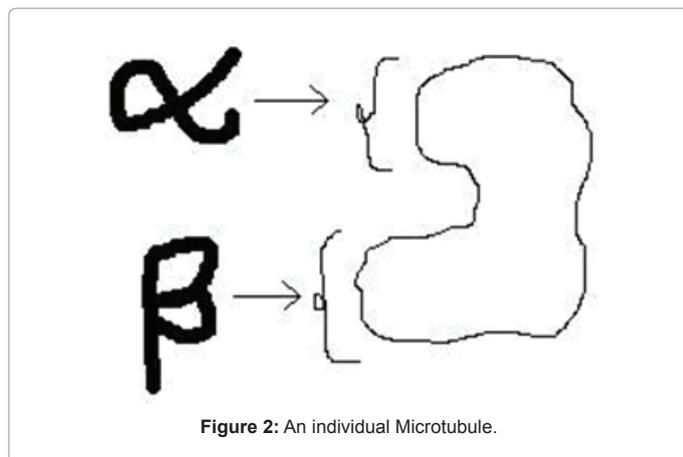


Figure 2: An individual Microtubule.

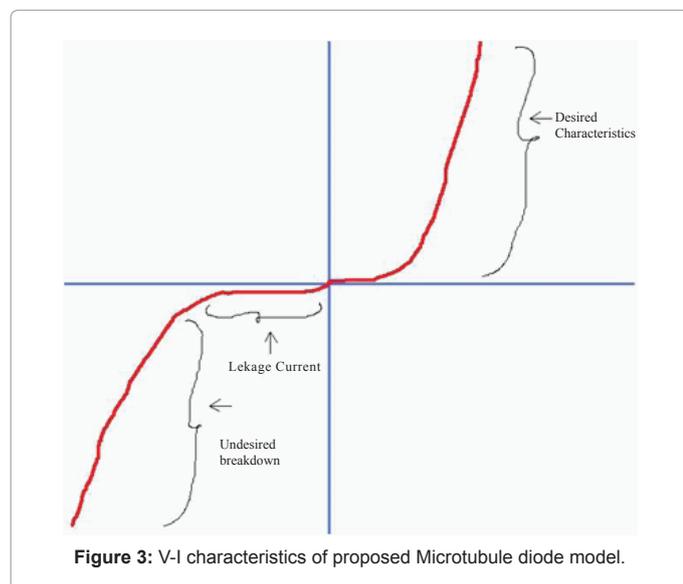


Figure 3: V-I characteristics of proposed Microtubule diode model.

### Modeling a diode from a mt

The idea to model a MT to act as a diode is from the tunneling phenomenon of the ions which take place in the dimers of the MT. Mostly a breakdown in the device occurs when there is a large flow of current by minority charge carriers. But this type of breakdown need not be expected in the proposed model as the charge carriers are only ions in this case. In quantum mechanical statistics we can represent the dimers as quantum wells of different potentials that are stacked one after the other constituting a series of quantum wells arranged like the same. The tunneling potential required to overcome the barrier wall is proportional to the diode knee voltage which starts the flow in forward bias. It is similar to the switching action that takes place in solid state devices.

The reverse bias is an action that does not work in the ion flow direction. So, the MT would behave ideally like a diode. The ion flow is said to take place in unidirectional manner, so the other direction current flow is very less. Therefore, ideally no conduction is said to take place in the reverse bias. Electronic comparisons of the MT with electronic variation of a solid state semiconductor diode can be quoted as: 1. The doped semiconductor, unlike in a diode, can be compared with the two dimers, alpha and beta, of the MT filament 2. It is only after a threshold potential, the flow starts and the same decides the knee voltage of the biomolecular MT diode.

### The quantum mechanical conduction profile equation of an mt

Mapping of the MT into a one dimensional quantum well is done to take the conduction profile of the MT. This is done to visualize the proposed model for modeling a diode from two MT molecules. Quantum mechanics has been followed to check the conduction of the MT since the dimension of a single MT molecule is in the range of a few nanometers. Classical physics fails to explain its conduction in discreteness. In the proposed model the tunneling phenomenon is observed by the ion transfer from one dimer of the MT molecule to the other dimer of the next adjacent MT molecule. Figure 4 is the one dimensional potential well with their energy profile. The tunneling of the ions in the wells by diffusion is explained using the Hamiltonian statistics in equation [2]. Current density through the dimers is estimated in the tunneling current that traverses through the ion channels in them. The current equation for it is in equation [3]. The equation is a function of the probability given by the tunneling phenomenon. The probability (P) is given by the quantum mechanical statistics. By the comparison and equating the diffusion equation as a phenomenon of ion current flow in the model the tunneling current equation is established in between the dimers, the diode model is benefited from a MT molecule.

$$J_n = q (\mu n n E + D n (dn/dx))$$

equation 2. Diffusion current density.

$$J_n = q V_r n P$$

equation 3. Tunneling diffusion current density.

The proposed model design considers a pair of MT molecules in which the ion transfer would describe its working as a diode in all characteristics. Tunneling current is solved from the time independent Schrödinger wave equation given in equation [4]. The Schrödinger time independent wave equation is used to solve it since the motion here is only potential dependent and then there is no need of time space. Solving the Schrödinger equation we get the probability parameter (P) of the tunneling current. The solved probability from the Schrödinger equation is in equation [5]. By analyzing both the ion flow equations, it has been found that the dimer molecule pair can act as a diode in all its characteristics.

$$(-\hbar^2/2m^*) (d^2\Psi/dx^2) + V(x) \Psi = E\Psi$$

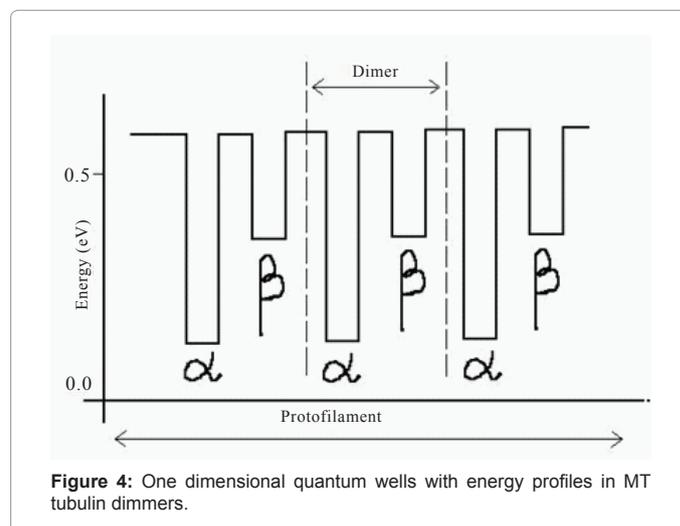


Figure 4: One dimensional quantum wells with energy profiles in MT tubulin dimmers.

equation [4]. Time independent Schrödinger wave equation.

$$P = \exp \left\{ \left( -\frac{4}{3} \right) \left[ \sqrt{2qm^*} / \hbar \right] \left[ \phi b (3/2) / \epsilon \right] \right\}$$

equation [5]. Probability parameter solved for tunneling ion current density.

Previously research work has been done to check the parameters needed to control the biomolecule from degrading and conduct the ion current flow [1] [2]. Analysis has also been done in the application of the solid state physics in biological molecules and biological systems [3]. Modeling of the devices in the nano level by using biomolecules and biological systems are innovations being followed to replicate the property of biomolecules to make an impact in the biocompatible electronic devices. This nanobioelectronics is the current need for the modeling of these devices as per the solid state physics equivalents.

### Simulated section of ionic conduction

Based on the other nanobioelectronic device modeling references, some simulation work was done to analyze the practical implementation strategies as follows:

1) Simulated ion conductivity characteristics of a MT in consideration of temperature, specific conductivity and activation energy in reference to theoretical estimation of conductivity of biomolecules [4]. The simulated output is in figure 5. It explains the exponential conductivity characteristics of biomolecules.

2) Observed curves of conduction of the biomolecules in consideration of density of the charge carriers [5] [6]. Solid state physics is dependent on the density of the charge carriers as explained in this part of simulation result. The simulated observation is in figure 6.

3) A diode characteristic simulation result in consideration with temperature, current rating, bias voltage and saturation current for a MT. The simulated work of the proposed device to be modeled is in figure 7. For, the biomolecules, the temperature is also a parameter to be concerned with, as the thermal excitation of the ions [7] [8] has an influence in the ion excitation and charge conduction.

### Observation

Depending upon the medium present the conduction characteristics of the biological molecules vary. This confirms that the system is totally electrochemically dependent in signal flow. The activation energy

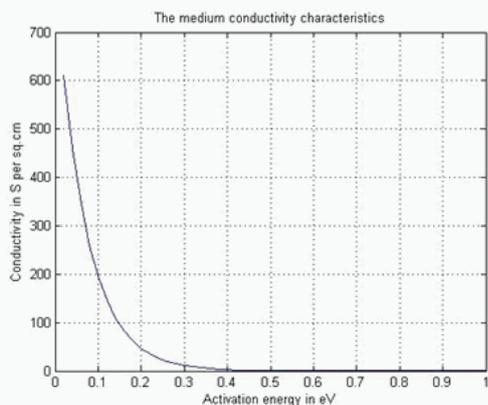


Figure 5: One dimensional quantum wells with energy profiles in MT tubulin dimers.

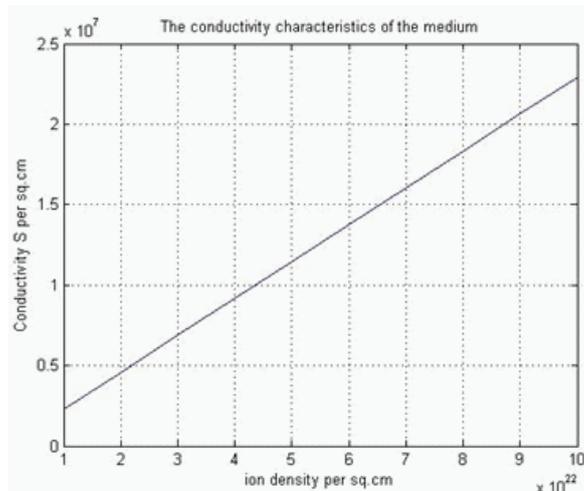


Figure 6: One dimensional quantum wells with energy profiles in MT tubulin dimers.

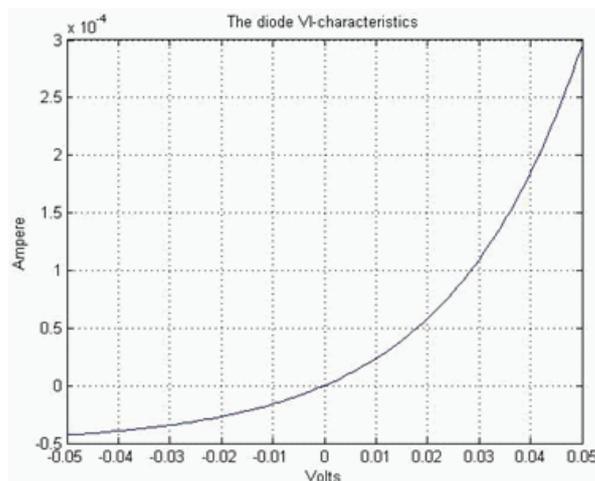


Figure 7: One dimensional quantum wells with energy profiles in MT tubulin dimers.

of the ions is dependent on the temperature as the thermal vibrations give them the required excitation. Hence modeling of devices from the biomolecules is possible when the molecules are not disturbed from their environment and are directly utilized. The diode model proposed is also favorable in using the MT molecule.

### Conclusion

In this paper, a modeling of a nanobiodevice, a diode was theoretically analyzed. The method to increase the stability of its working has been discussed and it was found to be assertive.

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