Towards Protein-Based Bio-Electronic Circuit Components

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Abstract

In recent years, basic chemical methods have been designed for bottom-up synthesis of nanoscale materials. Among them are sol-gel processing, precipitation-, solvent evaporation and vapor phase reactions. The use of biological molecules offers exciting alternatives to the conventional synthetic methods. Specific methods use various biological templates to direct the deposition and patterning of inorganic materials. Our working hypothesis is that microtubules (MTs) and actin filaments play an active role in subcellular computation and signalling via electronic and protonic conductivity and thus can be made useful in hybrid materials that offer novel electronic characteristics. We verify these hypotheses both computationally and analytically through a quantitative model based on the atomic resolution structures of the key functional proteins. MTs and some associated proteins (MAP's) are ubiquitous cellular structures of eukaryotic cells important for organising cytoplasmic properties and cellular involvement. They are hollow protein filaments with outer diameters typically of ~25nm and inner diameters of ~15nm and are made of α β-tubulin dimers [1] (α- and β-subunit heterodimers associate into protofilaments). MTs typically consist of 13 protofilaments. The C-terminal regions of tubulin are important in the regulation of MT assembly, as attachment points for MAPs and are also involved in the docking and binding of motor proteins, e.g. kinesin. Stabilization of MTs by MAPs plays a role in informational processing of neuronal microtubules.

MTs have significant electronic properties due to the permanent electric dipole moment of tubulin and the negatively charged tubulin carboxyl-termini. Electric fields can transport suspended microtubules into a desired direction and steer microtubules actively driven by motor proteins. In vitro experiments showed [2] that individual MT's move steadily towards the positive electrode. Electrophoretic mobility decreases with ionic strength and pH. Microtubule movement changes direction to the anode at pH 4.1 indicating a positive net charge. Interpolation of the isoelectric point gives a value of about pH 4.2 for microtubules which is remarkably lower than that of α- and β-tubulin monomers found to be near pH 5.5. Nanometallic particles templated to produce bio-assemblies have potentially useful electronic properties due to their nanoscopic size, shape, and spatial distribution that can be controlled by physical and biochemical means [3,4]. The surface of tubulin molecules exposes a defined pattern of amino acid residues that provides active sites for nucleation, organization, and binding of metal particles. For the crystal structure of tubulin it has been shown that histidines are centrally located at both the α- and β-tubulin outer surface and they can be regarded as nanoparticle binding sites. Under appropriate conditions, every tubulin molecule is able to nucleate and to bind silver, gold, platinum and palladium nanoparticles thus forming regular arrays reflecting the tubulin array patterns in an isomolecular fashion. By further particle growth, a quasi-continuous microtubule coating can be obtained resulting in metallised nanowires and furthermore these wires can be assembled into circuits. Such an isomolecular organization of nanoparticles into functional 2D and 3D structures provides a potential approach to develop electronic devices with novel I-V characteristics and attractive physical and biochemical properties such as self-organization and ease of manipulation. Bio-macromolecular assemblies offer a great potential to develop novel inorganic materials useful for electronics, information processing, and catalytic processes.

Using a variety of computational techniques we have examined theoretically the protein tubulin which assembles into MTs and the globular form of actin and its double stranded filaments. We have undertaken transmission line modeling [5], for MTs with different lattices as well as microtubule-

associated protein (MAPs) that together with MTs form networks. Electronic conductivity calculations for the bare MT structure have been based on the Hubbard model in which the dynamic conductivity matrix has been determined using the Kubo formalism in conjunction with the periodic square well approximation, reflecting the lattice geometry. We have investigated MTs decorated with metallic nanostructures using a percolating resistor network approach where metallic wires are interconnected with protein segments represented as insulators with resistance values we have calculated earlier. In particular we have carried out computations of the I-V characteristics of metallized MTs. Our first step was a detailed computation of the 3D crystal structure of each protein and its electrostatic properties utilizing the atomic resolution PDB files for tubulin and actin. This was then used to determine their electric potentials, charge distributions and dipole moments which are then extended to their respective filaments.

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