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High-Fidelity Modeling, Heterogeneous Simulation and Optimization of Synchronous Nanomachines and Motion Nanodevices

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Abstract — Rotational and translational nanomachines, controlled by nanoscale integrated circuits (nanoICs), can be widely used as actuators and sensors. The implications of nanotechnology to motion nanodevices have received meticulous consideration as technologies to fabricate these nanomachines have becoming developed. In particular, organic and inorganic micromachines (fabricated using CMOS and micromachining technologies), that serve as nanomachine prototypes and prove-of-concept paradigm, have been tested and characterized. In this paper we address and solve a spectrum of problems in synthesis, analysis, modeling and control of nanoscale permanent-magnet synchronous machines. All nanomachines and motion nanodevices must be synthesized before attempts to design and optimize them because basic physical features, nanomachine topologies, energy conversion, operating principles and other issues significantly contribute to sequential tasks in analysis, control, optimization and design. This is of particular significance for electromagnetic motion nanodevices including permanent-magnet synchronous nanomachines. This paper illustrates that depending upon the distinct analysis methods, different results are obtained. The fundamental, applied, and experimental results reported illustrate the validity and effectiveness of the results.

Keywords — nanodevices, nanomachines, nanotechnology

I. INTRODUCTION

The benchmarking problems in the synthesis of novel high-performance nanomachines have challenged academia, industry and government laboratories. Though some progress has been made in nanobiomotors [1, 2], many unsolved problems exist in devising inorganic nanomachines [1, 3, 4]. As a result, new solutions are sought. Therefore, it is a strong interest to design novel nanomachines controlled by nanoICs.

We document novel results in synthesis of electromagnetic nanomachines with the corresponding modeling, simulation, analysis and optimization tasks. In this paper, to attain the highest degree of integrity, high-fidelity models are developed and examined. A wide spectrum of interactive software tools, algorithms and programs have been developed to solve these long-standing problems in heterogeneous simulation and data-intensive analysis. The optimization problem should be solved to guarantee the superior overall performance of nanomachines. Using the developed high-fidelity mathematical models of synchronous nanomachines, the simulation results illustrate the efficiency of the modeling, analysis and optimization methods. In addition to applied and fundamental research, the experimental results are performed. The prototype of the reported axial topology nanomachine is designed and fabricated. This micromachine with deposited nanomagnets is tested and characterized. This provides the evidence that affordable high-performance axial topology nanomachines can be designed, fabricated and deployed.

II. SYNCHRONOUS NANOMACHINE SYNTHESIS

We consider the nanobiomotor of E.coli bacteria. The flagella (rotated by nanobiomotors) are used for propulsion. The bacterium is propelled with maximum speed 20 μm/sec by flagellar filaments. This filament is driven by a 45 nm rotor of the nanobiomotor embedded in the cell wall. The cytoplasmic membrane forms a stator. This nanobiomotor integrates more than 20 proteins and operates as a result of the protonomotive force resulting due to the proton flux. The rated nanobiomotor parameters were found to be [2]: angular velocity is 20 rad/sec, torque is 1x10^{-16} N-m, and efficiency is 50% (estimated). The nanobiomotor has three switch proteins (FlhG, FlhM and FlhN) that control the torque, angular velocity and direction of rotation. These proteins are involved in the flagellar assembly. It was found in [2] that FlhG interacts with FlhM, FlhM interacts with itself, and FlhM interacts with FlhN. The flagellum, flexible joint (proximal hook) and nanobiomotor are shown in Figure 1 [2, 3]. The nanobiomotor has two major parts, e.g., a stator (connected to the cell wall – peptidoglycan) and a rotor (connected to the flagellar filament through flexible joint).
Figure 1. E.coli nanobiomotor, nanobiomotor – coupling – flagella complex with different proteins and rings, rotor image, and possible protein-based bionanocircuitry geometry

The stator is built using the so-called MotA and MotB complexes, while the rotor is built by FlfF, FlgI, FlgM and FlgN protein forming the so-called MS and C rings. The shaft is made from proteins FlgB, FlgC, FlgF and FlgG, while the protein is built from proteins FlgH and FlgI forming the so-called L and P rings. The MS, P and L rings each contain many copies of FlgH, FlgI and FlgN proteins, respectively. Paper [2] reports that there are eight stator elements (MotA and MotB complexes) each of which exerts the same force. The torque is developed due to axial flux of protons (only in marine bacteria that live at high pH the sodium ions establish the axial flux). The source of energy is a transmembrane electrical potential and/or pH gradient. MotA and MotB complexes form a transmembrane channel. According to [2], proton translocation may cause the cytoplasmic part of MotA to move or change the geometry, producing the force on FlgG. The motor rotates clockwise or counterclockwise, and the change of the direction results due to proteins FlgI, FlgM and FlgN. When the nanobiomotor rotates clockwise, the flagellar filaments work independently, and the cell body moves erratically with little net displacement (bacterium tumbles). When the nanobiomotor rotates counterclockwise, the flagellar filaments rotate in parallel in a bundle that propels the cell body forward (bacterium runs). There are multiple copies of proteins that build the flagellum, and, as an example, there are thousands of FlfC molecules per helical turn of the filament which has up to six turns.

The analysis of nanobiomotors is far from completeness, and there is a significant lack of reliable data [2]. There are a couple of possible torque production and energy conversion mechanisms that lead to the corresponding operation of electromagnetic nanobiomotor:

- **synchronous electromagnetics** – the torque results due to the interaction of time-varying magnetic field established by the stator (rotor) windings and stationary magnetic field established by the rotor (stator) permanent nanomagnets;
- induction electromagnetics – the rotor currents are induced in the rotor windings due to the time-varying stator magnetic field and motion of the rotor with respect to the stator, the torque results due to the interaction of time-varying electromagnetic fields;
- variable reluctance electromagnetics (synchronous nanomachine) – the torque is produced to minimize the reluctance of the electromagnetic system, e.g., the torque is created by the magnetic system in attempt to align the minimum-reluctance path of the rotor with the time-varying rotating airgap mmf.

With the limited knowledge available to date, one can hypothesize that the E.coli nanobiomotor operates based upon the synchronous electromagnetics. With the high degree of confidence it can be concluded that the electromagnetic system is closed and nanomotor has an axial topology (nanobiomotors use the proton or sodium gradient, maintained across the cell’s inner membrane as the energy source, and the torque is developed due to the axial flux). Complex chemo-electro-mechanical energy conversion is a far-reaching research that unlikely will be completed in near future. It is extremely difficult to comprehend and prototype the torque generation, energy conversion, bearing, sensing-feedback-control and other mechanisms in nanobiomotors.

Despite the limited research and evidence, efficient nanomachines can be synthesized utilizing the axial topology and endless electromagnetic system. In fact, high-performance axial topology micromachines have been synthesized, designed, tested and characterized [3, 4]. Though these nanomachines are different compared with the E.coli nanobiomotor which may not have permanent magnets, the similar topology is utilized. Furthermore, we progressed to the well-defined and well-understood inorganic motion nanodevices that can be fabricated utilizing nanotechnology, micro-machining technology and modified CMOS processes.

The advantages of axial topology nanomachines are efficiency and reliability. Fabrication simplicity result because: (1) nanomagnets are flat, (2) there are no strict shape requirements imposed on nanomagnets, (3) rotor back ferromagnetic material is not required, and (4) it is easy to deposit planar nanowires on the flat stator. Utilizing the axial topology and endless electromagnetic system, we synthesize permanent-magnet synchronous nanomachines. The synthesized nanomachine is reported in Figure 2. This nanomachine has well-defined topological analogy compared with the E.coli nanobiomotor. It must be emphasized that the documented motion nanodevice can be fabricated, and a prototype of the micromachine with 40 \( \mu \)m rotor was fabricated and tested. The planar segmented nanomagnet array, as evident from Figure 2, can be deposited as thin films nanomagnets.
mechanical phenomena, is given as

\[ F = \rho_s(E + \nabla \times B) = \rho_s E + J \times B. \]

The electromagnetic force is found applying the Maxwell stress tensor. This concept employs a volume integral to obtain the stored energy, and

\[ F = \int (\rho_s E + J \times B) \, dv = \frac{1}{\mu_s} \int T_s \, ds, \]

where the electromagnetic stress energy tensor is

\[ T_s = T_e + T_m \]

\[ = \begin{bmatrix} E_1 D_1 - \frac{1}{2} E_2 D_2 & E_1 D_2 & E_1 D_3 \\ E_2 D_1 & E_2 D_2 - \frac{1}{2} E_3 D_3 & E_2 D_3 \\ E_3 D_1 & E_3 D_2 & E_3 D_3 - \frac{1}{2} E_1 D_1 \end{bmatrix} \]

\[ + \begin{bmatrix} B_1 H_1 - \frac{1}{2} B_2 H_2 & B_1 H_2 & B_1 H_3 \\ B_2 H_1 & B_2 H_2 - \frac{1}{2} B_3 H_3 & B_2 H_3 \\ B_3 H_1 & B_3 H_2 & B_3 H_3 - \frac{1}{2} B_1 H_1 \end{bmatrix} \]

For two regions (airgap \( ag \) and permanent magnets \( pm \)), we have the airgap and permanent magnet flux densities as

\[ B_{ag} = \mu_0 H_{ag}, \]

\[ B_{pm} = \mu_0 H_{pm} + J = \mu_0 (\mu_r H_{pm} + M), \]

where \( M \) is the residual magnetization vector, \( M = B_0 / \mu_0 \mu_r \); \( B_0 \) is the remanence; \( \mu_r \) is the relative recoil permeability.

The negative gradient of the scalar magnetic potential \( V \) gives the magnetic field intensity, e.g.

\[ H = -\nabla V. \]

The scalar magnetic potential satisfies the Laplace equation in free and homogeneous media (with zero current density, e.g., \( J = 0 \)).

For axial topology nanomachines, the cylindrical coordinate system is used. We have

\[ \nabla \cdot M = \frac{1}{r} \frac{\partial (r M_r)}{\partial r} + \frac{1}{r} \frac{\partial M_\phi}{\partial \phi} + \frac{\partial M_z}{\partial z}. \]

Solving the partial differential equation [5]

\[ 1 + \chi \frac{\partial^2 V}{\partial r^2} + \frac{1 + \chi}{r^2} \frac{\partial^2 V}{\partial \phi^2} + (1 + \chi) \frac{\partial^2 V}{\partial z^2} = \nabla \cdot M, \]

the three-dimensional airgap flux density is found as

\[ B_{ag} (r, \phi, z) = \left( \frac{\mu_0 M_0}{1 + \chi} \right) \sum \frac{\sinh \frac{\nu \phi}{r}}{1 + \chi} \frac{\sinh \frac{\nu z}{r}}{1 + \chi} \frac{\nu \phi}{r} \]
where $\chi$ and $\chi'$ are the reversible susceptibility along the easy and transverse magnetization axes; $a_i$ is the harmonic amplitude coefficient, and for the trapezoidal-wave magnetization, $a_i = \frac{4\sin(2i-1)}{\pi(2i-1)^2}$; $h_i \leq z \leq g_{ai} + h_i$, $h_i$ is the rotor thickness.

One-dimensional airgap flux density is found to be

$$B_{ag}(\phi) = \frac{\mu_0 M_i h_i}{(1 + \chi)(h_i + g_{ai})} \sum a_i \sin \nu \phi.$$  

The maximum flux density in the airgap is

$$B_{max} = \frac{\mu_0 M_i h_i}{(1 + \chi)(h_i + g_{ai})} \sum a_i (-1)^{\nu}.$$  

Using the derived equations for the airgap flux and emf

$$emf = \int E \, d\phi = -\frac{\partial B}{\partial z} \cdot d\phi,$$

one finds three-dimensional electromagnetic model for nanomachines dynamics, torque production, and vibration. It should be emphasized that the electromagnetic torque is

$$T = m \times B.$$  

The radiated pressure $p(r, \theta, \phi, t)$ is found using the Green function $G$. We have

$$p(r, \theta, \phi, t) = \rho \int_{0}^{2\pi} \int_{0}^{\pi} \omega(\phi, z) G(r, \theta, \phi) \, d\phi \, dz.$$  

The developed equations of motion model electromagnetic – mechanical – vibroacoustic behavior of synchronous electromagnetic nanomachines.

IV. OPTIMIZATION OF NANOMACHINES

We propose the design paradigm to guarantee optimal electromagnetic, mechanical and vibroacoustic behavior of nanomachines. The electromagnetic and mechanical design are based on the application of Maxwell's equations and tensor calculus in order to optimize the complex electromechanical behavior in nanomachines. For example, the nanomachine components (magnets, windings, air gap, etc.) geometry can be optimized to maximize efficiency ($\eta$) and robustness as well as minimize torque ripple and losses. In addition to the passive optimization, the active optimization – control problem is formulated and examined. The mathematical formulation of the active optimization – control problem is given as

$$\text{max min} \{ \eta, T, p(t, r, \theta, \phi), \}$$

where $u$ is the control vector. Different control variables can be used. For axial and radial topology synchronous nanomotors, the electromagnetic field is controlled varying applied voltage.  

V. EXPERIMENTAL RESULTS AND VALIDATION

High-fidelity modeling, heterogeneous simulation, data-intensive analysis and optimization have been performed for a 100 nm diameter axial nanomachine. The fundamental results have been verified for the fabricated micromachines. The electromagnetic field, electromagnetic torque, angular velocity, vibration, noise spectra and other variables for different axial topology motion devices have been measured and analyzed. The optimized and computationally efficient MATLAB files are developed to perform a coherent analysis. These experimental results validate fundamental research documented in this paper.

VI. CONCLUSIONS

The major objectives of this paper were to (1) devise and synthesize permanent-magnet synchronous nanomachines, (2) derive high-fidelity mathematical models, (3) perform electromagnetic-vibroacoustic analysis, (4) solve the active optimization – control problem, and (5) validate the results. Axial topology permanent-magnet synchronous nanomachines were synthesized. It is very important that these nanomachines can be fabricated expanding the existing technologies. Accurate assessment of nanomachine performance depends upon mathematical models used in design and analysis. Therefore, a complete high-fidelity mathematical model of synchronous nanomachines was developed, and electromagnetic-vibroacoustic phenomena were examined. The major goals were to maximize efficiency, guarantee robustness, reduce vibration, attain affordability, etc. It is necessary to devise, assess and accurately analyze nanomachines. One also needs to perform the electromagnetic-mechanical-vibroacoustic design to optimize electromagnetic-electromechanical systems. Therefore, the integrated electromagnetics-electromechanics was examined. In fact, simplifications, assumptions and disintegration made applying the lumped-parameter and finite element analysis methods do not allow one to perform accurate analysis and optimal design. The developed mathematical models were validated and applied to perform analysis, optimization and assessments of synchronous electromagnetic nanomachines.

REFERENCES