A Multiphysics Modeling of Electromagnetic Signaling Phenomena at kHz-GHz Frequencies in Bacterial Biofilms

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ABSTRACT This paper presents a model that describes a possible mechanism for electromagnetic (EM) signal transmission and reception by bacterial cells within their biofilm communities. Bacterial cells in biofilms are embedded into a complex extracellular matrix containing, among other components, charged helical nanofibrils from amyloid-forming peptides. Based on the current knowledge about the nanoscale structure and dynamics of the amyloids, we explore a hypothetical model that the mechanical vibration of these nanofibrils allows the cells to transmit EM signals to their neighboring cells and the surrounding environment. For the reception, the induced electric field can either exert force on the charges of adjacent nanofibrils associated with the neighboring cells or affect the placement/conformation of a certain charged messenger protein within the cell. The proposed model is based on a coupled system of electrical and mechanical nanoscale structures, which predicts signal transmission and reception within kHz-GHz frequency ranges. Different mechanisms for generating EM signals at various frequency bands related to the structure of the cell and their biofilm constituents are discussed.

INDEX TERMS Biological cells, electromagnetic signaling, quorum sensing, coupled resonators, biofilms, multiphysics modeling; amyloid nanofibers.

I. INTRODUCTION

Biofilms represent communities of numerous microorganisms typically including bacteria and fungi [1]. They form and grow in different parts of the Earth ecosystems as well as clinical and industrial settings. The human body hosts biofilms in the mouth, skin, lungs, and intestinal tract that can protect our health or harm it depending on their microbiological composition [2]. Bacterial biofilms are responsible for a majority of clinical infections [3] posing a serious threat to public health due to their tolerance to antibiotics compared with individual bacteria [4]. Hence, understanding the characteristics of biofilms under diverse conditions is of great importance.

The proper function and survival of bacterial communities depend on the ability of individual cells to communicate with each other [5]. The critical parameters that cells need to sense and process include their own density and microbial composition of the biofilms [6]. Cells can adjust their gene expression in response to information received from adjacent cells by means of chemical signals (autoinducers) that reach adjacent cells via diffusion [7], which is the commonly accepted communication mechanism between bacterial cells known as quorum sensing (QS). For example, Gram-positive bacteria, such as Staphylococcus aureus, utilizes oligopeptides as chemical messengers [8]. Autoinducers let bacteria sense population density and change their behavior in a synchronized fashion when the density reaches a certain threshold. Bacterial populations will activate or inhibit specific genes only when they are able to sense that their population is numerous enough [9]. Recent experimental investigations indicate that some biofilms take advantage of spatially propagating waves of charged potassium to coordinate their...
metabolic states as well as to synchronize their growth dynamics with other distant biofilms [10], [11]. It should be noted that all the above-mentioned communication schemes rely on the diffusion of molecules and ions, which limits the communication range and response time.

A better understanding of communication methods of bacteria within the dense and diverse community of cells in biofilms to coordinate metabolic states among themselves, is needed for controlling biofilm for biomedical, technological and environmental needs. There is a hypothetical but intriguing possibility that in addition to chemical signaling using autoinducers and ion channels, bacterial cells can also transmit/receive electromagnetic (EM) waves. We may need to consider this possibility because there is a growing body of evidence that low-energy electromagnetic phenomena associated with the kHz-THz range of frequencies take place in biological systems. As such, latest studies show some bacterial DNA sequences emit electromagnetic waves (~kHz) at high aqueous dilutions after excitation by the ambient electromagnetic background [12], [13]. Microtubules in the cytoskeleton of eukaryotic cells are also conjectured to emit time-varying electric fields (~GHz) through mechanical vibration of their tubulin monomers having permanent dipole [14], [15]. However, no experimental evidence has confirmed these high frequency oscillations. Similarly, proteins, their assemblies and other biological materials have demonstrated high frequency oscillations and spectral resonances at around THz frequency [16]-[18], which can be the source of EM emission and absorption. Besides natural THz emission by biological organs, the THz frequency band has also been examined extensively for intra-body communication networks and sensing applications [19], [20]. This is mainly due to the available bandwidth and the relatively small wavelength size which can be leveraged to realize efficient nano-scale antennas utilizing surface plasmonic concepts and novel materials including graphene [21].

Among many biological systems, bacterial biofilms can be a convenient experimental and theoretical system for evaluating the possibility that these organisms can transmit and receive EM waves as a means of communication [22]-[24]. While this hypothesis was discussed in the past, there is no compelling experimental evidence or a plausible biophysical mechanism associated with such conjecture to date. To further motivate this investigation, it is important to make a comparison between the proposed EM based communication in biofilm and the conventionally accepted QS. This will indicate why EM signaling can complement or even enhance inter-cell communication at least in some instances. For that purpose, we have recently developed a communication channel model comparison between EM signaling and QS indicating that EM signaling can provide orders of magnitude higher data rate when compared with QS [23].

Let us consider the biological nanoscale structures of the environment constituting biofilms to understand better from where and how EM emission may originate. Fig. 1(a) illustrates a scanning electron micrograph of an *S. aureus* biofilm. Cells in a biofilm are embedded in an extracellular matrix of hydrated polymeric substances (EPS) [25]. The major matrix components are polysaccharides, lipids, DNA segments and proteins some of which can form amyloid fibers. The EPS matrix provides mechanical stability for biofilms, mediates their adhesion to surfaces and interconnects biofilm cells through the formation of a three-dimensional network. In addition, EPS acts as an external digestive system by keeping extracellular enzymes in close proximity to the cells, enabling them to metabolize dissolved, colloidal and solid biopolymers [26]. Amyloid nanofibrils represent a common nanoscale component of the EPS matrix of many types of bacterial biofilms and specifically those produced by *S. aureus*, and *Bacillus subtilis* serving as common biofilm models. In the framework of this study, amyloid nanofibrils can be described as elastic helical fibers carrying a negative charge [27]-[29]. The amyloid nanofibrils are produced by the self-organization of peptides and proteins [30], [31] undergoing in this process a change of configurational states. For instance, amyloid nanofibrils in *S. aureus* biofilms are self-assembled from peptides known as phenol-soluble modulins (e.g., PSMα, PSMβ) [32]. The self-assembly process of PSMs into nanofibers involves backbone hydrogen bonding and side-chain interaction (e.g., hydrophobic interaction, π-stacking, and van der Waals attraction) [33], [34]. The individual peptides have distinct dipole moment oriented along the direction of the alpha helix, mostly due to their barrel-like structure and zwitterionic state. While the detailed atomistic structure of the peptides in amyloid fibers is not entirely clear, especially in transient forms, the complex curved shape of these nanostructures and stacking of the individual peptides in the fiber can give rise to uncompensated dipole moment [35]. As can be observed from Fig. 1(b) and Fig. 1(c), the nanoscale nanofibrils are either suspended within the biofilm environment or attached to the cell wall. We contend that the charged nanofibrils can vibrate due to thermal motions, variable stresses and potentially due to some metabolic processes and consequently they radiate detectable EM waves [36]. Thus, amyloid nanofibrils potentially play a role as nanoscale antennas capable of emitting and receiving the EM signals replicating some of the metallic and semiconducting assemblies [37]. Importantly, the mechanical and electrical properties of these antennas are coupled due to the strong dependency of the surface charges on the curvature of the nanoscale structures [38]. The frequency of communication is then governed by the modulus of elasticity, mass density, surface charge density, etc. of both cells and the amyloid nanofibrils as well as the biological interface between the fibers and cells.
In this paper, as an intermediate step, molecular dynamics (MD) simulations are first carried out to determine the permanent dipole moment of amyloid fibers in *S. aureus* biofilms. This result is presented in Section II, where it is demonstrated that amyloids formed from an ordered arrangement of peptides (see Fig. 2) present a permanent dipole moment [35], whose estimated value is corroborated against other reported values in the literature. Then to explore possible ways of electromagnetic signal generation by biofilms, in Section III, different vibrational modes for these charged fibrils, including spring mode and cantilever mode, are explored. Fundamentally, accelerated charges can radiate electromagnetic fields, hence fast vibrating charged fibrils can potentially act as the source and the antenna for cells in biofilms. A model based on an electromagnetically-coupled system of bio-mechanical oscillators is developed to evaluate the characteristics of this EM signal generated among the cells in a biofilm. Different mechanisms that lead to EM signal emission within the kHz-GHz frequency range are described. For EM communication among cells, such vibration must be initiated by the cell itself. Using COMSOL Multiphysics simulation tool, in Section IV, it is shown that sudden realistic deformation of the cell caused by the release of accumulated stress or some metabolic process, can excite internal resonant vibration which, in turn, cause vibrations of attached amyloid fibrils. Such motions and the generated EM waves exert force on the charges of adjacent amyloid fibrils or other charges within the adjacent cells. Within the framework of this paper, the emission of EM waves from such a model is being explored, while their reception and transduction into the biological signal remain hypothetical. Finally, Section V provides concluding remarks.

II. AMYLOID NANOFIBRILS AS SOURCE OF EM EMISSION

A. NANOFIBRIL FORMATION FROM CHARGED PEPTIDES: MOLECULAR DYNAMICS (MD) SIMULATION

Despite the variety of papers reporting on PSMa amyloid nanofibrils [39], [40], their structural information required
for this study, even for common *S. aureus* biofilms, remains limited. Particularly, the mechanism that describes the transformation from the α-helical non-aggregated PSMα1 peptides to the β structure that characterizes the mature amyloid fibers is still unclear. The timescale of this transformation, which can span from a few days to a few weeks depending on the presence of other species [41], [42], is indicative of a process involving multiple relatively stable intermediates. As it is unclear if only specific aggregates can be responsible for bacterial communication, we analyzed the properties (i.e., electric dipole and geometry) of different candidate aggregates of PSMα1 peptides in both α-helical and β-sheet structure. To this end, we used MD simulations to generate several plausible structures based on biological evidence and compared the properties of these structures with measurements of fibers generated from pure PSMα1 solutions [43] (Fig. 2(a)). Simulations were performed using Nanoscale Molecular Dynamics (NAMD) [44] and PLUMED [45] software and all-atom CHARMM force field parameters [46]. A cutoff of 1.2 nm was used in conjunction with the particle mesh Ewald method [47] to evaluate long-range Columbic forces. The systems were first minimized, then equilibrated using harmonic restraint between peptides in an isothermal-isobaric ensemble, where the temperature was kept at 310 K with a Langevin thermostat [48] and the pressure at 101.325 kPa with a Langevin piston method [49], [50]. After gradually removing the restraint, the systems were simulated for at least 100 ns, using the evolution of the RMSD of the assembly as the criterion to decide when to terminate the simulations. The final structures were then used as starting points for the production simulations.

All the stable simulated structures show a relatively large net dipole. For a single peptide (Fig. 2(a)) it is oriented along the alpha-helix (approximately $6 \times 10^{-28}$ C.m, or 180 D) with a wide distribution of intensities depending on the conformation (4.3-8.7$\times 10^{-28}$ C.m, or 130-260 D). The high value of the dipole is not surprising and should be considered fairly typical for a lot of nanoscale structures [51]. For the assembled structures, the electric dipole is oriented approximately along the direction of the fiber (see Fig. 2(b) for one example). While the details vary from structure to structure and depend on the organization of the fiber over several hundreds of nanometers, the angle between the dipole computed from the overall charge distribution and the average fiber direction is within 20°.

For the purpose of this work and to generalize beyond the scale limitations of the MD simulations, we computed an apparent charge as the ratio between the projection of the dipole along the fiber direction and the fiber length. For the assembly formed by two protofilaments, which approximately match the experimentally observed radius of 10-12 nm [52], [53], we computed an apparent charge between 3 and 4 elementary charges. This is in close agreement with what also reported in [29].

### B. SOURCE OF EM EMISSION

Based on these and other data discussed above, we represented the amyloid nanofibrils as elastic helical strings or beams [28] being either suspended within the liquid medium of the biofilm or adhered to the cells (Fig. 1(b)). These elastic-charged strings can then be set in vibration by either the EPS matrix itself or cell through a sudden motion generated from metabolic processes or sudden release of accumulated stress. Any vibrating (accelerating) charge radiates EM waves at frequencies related to the charge’s motion dependent on the natural mechanical resonances of the nanofibrils. Therefore, charged amyloid nanofibrils may play the role of mechanical antennas within biofilms [36]. Due to the small dimensions and large molecular mass of cells and amyloids, the fields generated by such motions are expected to fall within radio frequencies, rather than the typical atomic oscillations that fall into optical and infrared ranges. The amyloid nanofibrils with permanent dipole moment in biofilms present a typical length and diameters of about 1 μm and 10 nm, a typical linear mass density of

![Image](https://example.com/image.png)
**III. VIBRATIONAL MODES OF AMYLOID NANOFLIRLS**

**A. MECHANICS OF SINGLE AMYLOID NANOFLIRIL AND CELL**

In order to conceptually understand the motion of amyloid nanofibrils and find possible natural resonant frequencies (normal modes), we first performed a solid mechanics modal analysis on amyloid nanofibrils that are attached to a cell. In this analysis, COMSOL Multiphysics simulation tool is used and the results are shown in Fig. 3. Here, the cell is modeled as a solid sphere \((R=440 \text{ nm})\) with Young modulus \(E=200 \text{ MPa}\), Poisson’s ratio \(\nu=0.4\), and mass density \(\rho_{\text{cell}}=1000 \text{ kg/m}^3\) based on the data obtained by atomic force microscopy. The nanofibril is modeled as a solid beam with bending rigidity \(EI\) with \(E=0.8 \times 10^{-36} \text{ N.m}^2\) and linear mass density \(\rho=46.2 \text{ kDa/nm}\). The amyloid nanofibril is 1µm in length \((l)\) and 10nm in width based on the TEM microscopy data in Fig. 1(c) and prior studies of amyloid fibers in biofilms. In general, the nanofibril length can vary from 0.1µm to 6µm. Simulation results show that due to the flexibility of nanofibrils compared with the cell, at low frequencies, while the cell is stationary, they mainly undergo cantilever beam vibrational modes with multiple nodes depending on the mode of vibration. The first four cantilever beam modes are shown in Fig. 3(b). But, at higher frequencies, the higher order modes of cantilever beam with multiple nodes and ant-nodes, couples to the cell’s vibrational modes and a complex (combined) mode of vibration will form from the cell plus its amyloid nanofibril (the last two resonance modes in Fig. 3(b)). It should be noted that the deformations shown here are significantly exaggerated for demonstration purposes. We will discuss these complex modes in greater details later when intercellular communication is discussed.

**FIGURE 3.** (a) Representation of a bacterial cell and attached amyloid nanofibril modeled as a solid sphere and a beam for normal mode analysis. (b) Structural mechanics modal analysis on an amyloid nanofibril attached to the cell. At low-frequencies, cantilever beam vibrational modes are observed for the nanofibrils within the kHz-MHz range (the first four modes are only shown here). At higher frequencies (the last two modes), the cell’s vibrational modes will combine with the higher-order modes of the cantilever beam associated with the fibril and then complex mode configurations appear. The resonant frequencies calculated analytically are in agreement with COMSOL finite element simulations. It should be noted that the deformations shown here are significantly exaggerated for demonstration purposes.

\[ \rho = 46.2 \text{ kDa/nm}, \text{ and a modulus of elasticity of } E=5-50 \text{ GPa} \]

Modal analysis of the resonance for this structure (single fiber), reveals a resonant frequency within kHz-GHz range depending on the mode of vibration. These calculations are the focus of next section.

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\[
\omega_n = \pi^2 n^2 \sqrt{\frac{EI}{\rho l^4}}
\]

Here \(\omega_n=1.8, 4.6, 7.8, 11.0\) are constants associated with the first four modes. As indicated in (1), the resonant frequencies are inversely proportional to the square of length. Given the information on Fig. 3(b), very close agreement can be observed between these analytical values and COMSOL simulations. Fig. 4 also depicts the resonant frequency of an individual amyloid nanofibril as a function of its length for its possible first four modes predicting that the resonant frequencies fall within the kHz-MHz range.
Therefore, illustrated in Fig. 5(a), such amyloid nanofibrils can be treated as low-resonant frequency charged cantilever beams. It should be noted that the vibration frequencies are in fact, the possible frequency of EM signaling within the biofilm because any accelerating charge is radiating electromagnetic waves at the frequency of acceleration (vibration).

The resonant modes of isolated amyloid nanofibrils (not attached to any cells) can be found considering them as distributed spring-mass oscillators while having a permanent dipole moment as shown in Fig. 5(b). Since the dipole moment is not necessarily along the fibril’s main axis (as depicted in Fig. 2), two spring modes must be considered, 1) longitudinal spring mode, and 2) transverse spring mode. These vibrational modes are along and normal to the fibril main axis, respectively.

Considering an elastic amyloid nanofibril (modulus of elasticity, $E \sim 5-50$ GPa) [28], [61], with length $l$, cross-section $A$ (width $w \sim 10$ nm, height $h \sim 2$ nm) [52], [53] and distributed mass $m = \rho l$ its resonant frequency can be calculated approximately as,

$$f_{LS} \sim \frac{1}{2\pi} \left[ \frac{K}{m} \right] = \frac{1}{2\pi} \left[ \frac{EA}{ml} \right] = \frac{1}{2\pi} \left[ \frac{E \times (w \times h)}{\rho l^2} \right]$$

$$f_{TS} \sim \frac{1}{2\pi} \left[ \frac{K}{m} \right] = \frac{1}{2\pi} \left[ \frac{E \times (l \times h)}{\rho' l \times w} \right] = \frac{1}{2\pi} \left[ \frac{E \times h}{\rho' \times w} \right]$$

Here, $f_{LS}$ and $f_{TS}$ are the natural resonant frequencies of longitudinal and transverse spring modes, respectively. $K$ is the effective spring constant of nanofibrils for each mode. The application of (2) and (3) show that such mode of vibration can potentially induce EM fields mainly within gigahertz frequency range (0.1-50 GHz) depending on the nanofibril’s length and mode of vibration. As given by (3) and also shown in Fig. 6(b), the transverse spring mode’s frequency is around 10-50 GHz and is independent of amyloid nanofibril length. It should be noted that for this mode of vibration, the motion of opposite charges associated with each nanofibril are out of phase and thus their emitting EM fields would be in-phase. Also note that these oscillations will not be induced by metabolic processes as opposed to amyloids in the cantilever mode, but rather contribute to the characteristic EM resonance frequencies of the biofilm (see below).

B. AMYLOID NANOFIBRILS AS EM-COUPLED MECHANICAL OSCILLATORS

Within a small volume of biofilms, there may be numerous amyloid nanofibrils with various lengths. Based on what explained and also illustrated in Fig. 7, this would create a system of electromagnetically-coupled mechanical oscillators. In fact, the vibrating charges provide EM coupling between adjacent elastic nanofibrils treated as mechanical oscillators. Since strong EM coupling can potentially exist between nanofibrils, their vibration frequencies are not necessarily the vibration frequencies of the isolated nanofibrils due to the frequency bifurcation phenomena observed in coupled resonators [62]. Appendix A, and Appendix B provide a detailed analysis of the electromechanical coupled system and describe the method for the calculation of the resonant frequencies. In brief, this analysis indicates that for the spring mode, EM interactions relative to the stiffness of nanofibrils are not strong enough to provide coupling and synchronization between the adjacent nanofibrils. Therefore, the vibration frequencies of coupled nanofibrils will be mainly the same as the individual’s frequencies. However, for the cantilever beam mode, strong coupling exists relative to the equivalent stiffness for this mode and the natural vibration frequencies of nanofibrils community mainly occurs in the kHz-MHz frequency range. The effect of this coupling is the strong synchronization of cantilever resonators at certain frequencies that has an effect of enhanced motion (higher...
amplitude of deflections) of the bio-mechanical resonators at these specific frequencies. The more is the amplitude of motion, the higher is the electric field produced by the biofilm. It should also be stated that as the frequency of spring mode (GHz) and cantilever beam mode (kHz-MHz) are far apart from each other, these vibrational modes are decoupled.

FIGURE 5. (a) Amyloid nanofibril attached to a cell can be treated as a charged cantilever beam. The $E$ and $I$ account for the young’s modulus and second moment of inertia associated with the fibril. (b) An elastic amyloid fibril connected to the EPS matrix and not attached to any cells can be modeled as a charged spring. Since its dipole moment is not along the fibril’s axis, it can be decomposed into two modes, namely, longitudinal and transverse modes.


IV. MULTIPHYSICS MODEL OF EM COMMUNICATION WITHIN BIOFILM

A. EM COMMUNICATION HYPOTHESIS

So far, our modeling has been only focused on the vibration of charged nanofibrils as the origination of EM waves in biofilm samples. For EM communication; however, this vibration must be initiated from the cell itself. Based on our hypothesis summarized in Fig. 8(a), it is expected that once a transmitting cell sets an amyloid nanofibril to motion through resonant vibration, it provides EM signal transmission from that cell to its environment as well as its adjacent cells. For receiving mode, according to the reciprocity theorem, the transmitted signal will transfer the wave energy to mechanical energy by exerting force on the permanent dipole charges of other amyloid nanofibrils attached to the adjacent cells. In other words, the signal reception is accomplished in the reverse order, that is, the time-varying electric fields generated by cells exert force on the permanent charges on amyloid fibers connected to a receiving cell which is then sensed by the receiving cell. Through the mechanotransduction process [63], [64], the cell senses this mechanical stimulus and will convert it into a biochemical, intracellular response.

As the cell-nanofibril modal analysis predicted before, the cell can also undergo a mechanical deformation along with its attached nanofibrils at higher frequencies. As shown in Fig. 3(b), this deformation couples to the higher order cantilever modes of the amyloid nanofibril causing a high frequency oscillation. As a result of this, EM signal will be created at the frequency and harmonics of the cell’s resonant vibration frequencies. To find these possible resonant frequencies, a solid mechanics modal analysis is performed on an individual cell (Fig. 8(b)). Using the same mechanical characteristics of the cell as in section III.A, i.e. \( R=440 \text{ nm, } E=200 \text{ MPa, } \) cell’s Poisson’s ratio \( v=0.4 \) [56], and mass density \( \rho_{cell}=1000 \text{ kg/m}^3 \) and by applying the stress-free boundary condition on the cell’s membrane \( (\sigma=0) \) [65], the natural spheroidal modes of the cell and corresponding resonant frequencies can be obtained through solving the Navier’s wave equation [66],

\[
\left( \lambda + 2\mu \right) \nabla (\nabla \cdot \mathbf{u}) - \mu \nabla \times (\nabla \times \mathbf{u}) = -\omega^2 \mathbf{u} \tag{4}
\]

Here \( u(r) \) is the radial displacement of every point within the cell, \( \omega \) is the natural resonant frequency of the allowable mode, and \( \lambda \) and \( \mu \) are the shear modulus and Lamé’s first parameter, respectively, given as [66],

\[
\lambda = \frac{E}{(1 + \nu)(1 - 2\nu)} \quad \mu = \frac{E\nu}{(1 + \nu)(1 - 2\nu)} \tag{5}
\]

Fig. 8(b) depicts the first four spheroidal modes of the cell. As can be seen, the natural vibrational frequencies for a single cell are in the range of 200 MHz-1 GHz and the ellipsoidal mode (second mode) has the lowest possible frequency while the breathing mode (first mode) occurs at higher frequencies. Through numerical simulations using COMSOL Multiphysics, the modal analysis results are also verified, and close agreements are observed. Additionally, the natural resonant frequencies of the combined modes for the cell-nanofibril configuration in Fig. 3, are mainly governed by the natural resonant frequencies of the cell and not of the nanofibril.

B. MULTIPHYSICS SIMULATION OF COMMUNICATION

To elaborate on high frequency combined modes of vibration and visualize the concept of EM communication, COMSOL Multiphysics is utilized. As a simple example, illustrated in Fig. 9(a), two cells with their attached amyloid nanofibrils are considered with intercellular distance \( R_c=1 \) \( \mu \text{m} \). The cells and nanofibrils are molded as solid spheres, and solid beams with the aforementioned mechanical properties. The amyloid nanofibrils are 1 \( \mu \text{m} \) in length and are attached to the cells’ membrane. The transmitting cell (TX) is assumed to experience a sudden strain along the \( z \)-axis given as,

\[
\epsilon_z = \frac{\Delta R}{R} = 0.025 \times g(t) \tag{6}
\]

where \( g(t) \) is the time-domain representation of applied strain (see Fig. 9(b)). With the applied strain, the cell is stretched along the \( z \)-axis by approximately 20 nm with a pulse having full width at a half max (FWHM) of \( \sim 2 \) ns. The applied strain of 20 nm (2.5%) is in close agreement with the experimental values for the cell’s surface deformation reported in the literature [67], [68]. Additionally, since the natural resonant frequencies of the cell structure falls in sub-GHz band, the time scale of the applied strain should be within nanosecond ranges. The applied sudden strain that can originate from metabolic processes, excites different modes of oscillation and potentially initiates the communication. Consequently, the cell starts vibrating and in-turn transfers the vibration to the attached amyloid nanonanofibril. Given the fact that nanofibrils have opposite charges on their both ends, there would be two contributing electric fields in transmission mode \( \mathbf{E}_{total} = \mathbf{E}_{+q} + \mathbf{E}_{-q} \). Fig. 10(a) and Fig. 10(b) show the vibration amplitude of the transmitting amyloid nanonanofibril ends (point A and point B in Fig. 9(a)), denoted as \( d_A(t) \) and \( d_B(t) \), respectively. Importantly, one may expect that due to the viscosity of water in the biofilm, the vibration of nanofibrils and cells get damped quickly. To have a qualitative account for viscous damping, let us calculate the time-domain profile of each of the end’s vibration, \( d(t) \), the generated electric field by each of the nanofibril dipole charges from [69],

\[
E = \frac{q}{4\pi \varepsilon_r \varepsilon_0} \left[ \frac{3}{uz^2} \frac{d(t)}{r^3} + \frac{3}{uz^2} \frac{d(t)}{r^3} \frac{u_z}{u_r} d \right] \tag{7}
\]

Where \( q \) is the dipole charge of the nanofibril, \( \mathbf{r} \) is the observation point measured from the location of each of the dipole charges at rest and \( d \) is the vibration amplitude vector. \( u_r \) also represents the phase velocity. Keeping only
those terms proportional to \( \frac{1}{r^3} \) as we are dealing with the near-field components (dimensions within a biofilm sample are in the order of nm-\(\mu\)m and the frequency is within kHz-GHz range), the expression for the electric field is simplified as,

\[
E = \frac{q}{4\pi\varepsilon_0} \left[ \frac{3}{r^2} (\hat{r} \cdot \hat{d}) \hat{r} - \frac{1}{r^3} \hat{d} \right] d(r) \quad (8)
\]

This indicates that the intensity of the induced electric field is proportional to the vibration amplitude of the nanofibril and the dipole charge which is calculated to be around \(3e^- (4.8 \times 10^{-19} \text{ C})\). Also, the \(\frac{1}{r^3}\) in the near-field region is the dominant term with much stronger E-field components compared to the far-field \(\frac{1}{r}\) given that \(r < 1\mu\text{m}\). This stronger E-field results in stronger electric polarization within the biofilm helping the cells sense the EM signaling more accurately.

Setting nanofibrils dipole charges \([29]\) \(q = 3e^-\) \((e^-\) is the electron charge value\), Fig. 11(a) and Fig. 11(b) show the

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**FIGURE 8.** (a) Hypothetical transmitting (TX) and a receiving (RX) modes of EM emission absorption of bacterial cells. The vibration of charged amyloid fibrils caused by the cell will induce EM radiation. (b) Structural mechanics modal analysis on an individual bacterial cell (analytical and numerical simulation). The natural resonant frequencies of the first four modes are in the sub-GHz range. Close agreement between the analytical frequencies and COMSOL normal modes is achieved. The given values in the parenthesis are for the COMSOL simulation results. It should be noted that the deformations shown here are significantly exaggerated for demonstration purposes.
received electric-field by the RX cell at point $D$ and point $O'$ (see Fig. 9(a)), respectively. From this figure, one can readily observe that the generated $E$-field has a high quality factor (there are a notable number of oscillation cycles before the vibration is fully damped) emphasizing on the sustainable resonance phenomena in the medium. For signal reception, the induced electric field can either exert force on charges of receiving nanofibrils to be sensed by the corresponding cell or it can move certain charged messenger protein within the cell. In order to obtain the frequency spectrum of EM signal among the cells and find the possible communication frequencies, the FFT of the

![Electric field](image)

**FIGURE 9.** (a) 3D view of a bacterial cell with its attached amyloid fibril surrounded by water. The cell is experiencing an initial strain along the $z$ -axis which in turn start vibrating and moving the amyloid fibril. The center or the TX and RX cells are located at $O(0,0,0)$ and $O'(0,0,-1) \mu m$, respectively. (b) Time-domain profile of the applied strain to the cell.

**FIGURE 10.** Vibration amplitude of the transmitting fibril’s ends. (a) point A ($d_A(t)$). (b) point B ($d_B(t)$). For the definition of points $A$, $B$, refer to Fig. 9. All the points are assumed to be initially on the $xz$ plane.

**FIGURE 11.** Electric field sensed by the RX cell. (a): at point $O'$. (b): at point $D$. For the definition of points $O'$, and $D$, refer to Fig. 9. All the points are assumed to be initially on the $xz$ plane.
generated electric field is calculated and the result is plotted in Fig. 12. It shows that cells and amyloid nanofibrils can generate an EM spectrum that includes frequencies up to about 5 GHz. However, as the frequency gets larger, the signal intensity decreases drastically indicating that, based on this model, communication at frequencies below 2-3 GHz is more probable specifically at around 500 MHz.

One last thing to discuss here is the effective permittivity for the cells and their water background ($\varepsilon_r$) used in (7) and (8). Experimental studies indicate that biofilms have a concentration of $10^9$ cell/mL [70]. Assuming spherical cells with a radius ($r=440$ nm), a cell volume fraction of $f=3.56 \times 10^{-4}$ is achieved. Since cells are small spherical particles in water background, using the dielectric-mixing formula [71], it can be shown that the effective dielectric constant is almost equal to the background medium (water) which is set to be 81 for our analysis.

Finally, in order to summarize these modeling efforts for readers, Table 1 provides all the viable modes of fibril vibration and the corresponding range of resonant frequencies.

V. CONCLUSION

This paper presented a theoretical model combining MD and electromechanical computations suggesting how individual bacteria may transmit and receive electromagnetic waves. The fundamentals of the operation of embedded radios within cellular structures are based on nanoscale antennas. Permanent dipoles within and around biological cells can be accelerated at their natural resonant frequencies through the cell’s natural metabolic activities and radiate electromagnetic signals from KHz-GHz frequencies. Amyloid nanofibrils typical for S. aureus biofilms are considered here in details. Our calculations show that once one of the normal vibrational modes of amyloid nanofibrils are excited, it may induce EM fields that could be received by adjacent cells. For the reception, emitted EM fields will exert force on the dipole charges of neighboring nanofibrils or move protein molecules within the cell. The modeling results show that nanofibrils having cantilever beam mode of vibration generate EM waves within the kHz-MHz range, and their mechanical spring modes excite GHz signals. In addition, the GHz frequency range is governed by the mechanical properties of the cell itself.

APPENDIX A

In order to clarify the role of EM coupling among nanofibrils and understand how vibration of one nanofibril gets affected by the adjacent nanofibrils, according to Fig. 7, one of the nanofibrils is assumed to be initially disturbed from its resting positions, due to some metabolic changes or activities in a cell, and go into motion. Then, due to EM coupling other nanofibrils can also potentially go to motion and transfer the message in the medium. To examine this scenario, we have first considered the cantilever vibration mode. The Lagrangian technique which is the resultant of Hamilton’s principle is applied to the constituents in the medium. For a single cantilever beam with length $l$ the equation of motion can be calculated analytically. Considering its first mode of vibration, the vibration amplitude distribution along the beam is,

$$w(x, t) = (1 - \cos(\frac{\pi}{2l}x))y(t)$$

here, as defined in Fig. 5(a), $x$ is the representation of coordinate system along the beam and $y(t)$ takes into account the temporal behavior of transverse vibration which can be for example proportional to $\cos(\omega t)$ for an oscillatory case. The stored kinetic energy ($T$) and the stored strain energy ($U$) in the cantilever beam can be obtained from [72],

$$T = \frac{1}{2} \rho A \int_0^l w^2 \, dx = \frac{1}{2} \rho A \left(\frac{3\pi^2}{8} - \frac{8}{2\pi}\right) l y^2$$

$$U = \frac{1}{2} EI \int_0^l w'^2 \, dx = \frac{1}{2} EI \left(\frac{\pi}{2L}\right)^2 l y^2$$

where $EI$ is the bending rigidity of the beam (nanofibril), $l$ is the length, $\rho$ is the volumetric mass density ($\rho = \rho A$) and...
A is the beam’s cross section. $\dot{w}$ is the time-derivative of $w(x,t)$ and $w''$ is the second derivative of $w(x,t)$ with respect to $x$. Now, back to our original problem with many anchored nanofibrils (Fig. 7(b)), defining the orientation of each nanofibril at its rest as $\phi_i$, and the amplitude of transverse oscillation of its open end as $y_i$, and considering the first mode of cantilever beam for each nanofibril, the Lagrangian of the system ($N$ nanofibrils) can be written as [73],

$$L = T - U - U_{EM} = c_{hyd}^y \sum_{i=1}^{N} \frac{1}{2} \rho_i A_i \left( \frac{3\pi}{2\pi} \right) l_i \dot{y}_i^2 - \frac{1}{4} \sum_{i=1}^{N} \sum_{i \neq j}^{N} \kappa_{ij} y_i y_j (12)$$

where, the first term accounts for the stored kinetic energy of the system, the second term includes the stored potential energy in the system and the third term which is the key element in describing electromagnetic-based communication, represents the dipole-dipole interaction of adjacent nanofibrils (electromagnetic potential energy, $U_{EM}$). As the induced EM signal wavelength (kHz-GHz) is considerably longer than typical dimensions within a biofilm (nm-µm), $\kappa_{ij}$ can be found using quasi-static approximations [74].

$$\kappa_{ij} = \frac{1}{2} \frac{q_i q_j}{4\pi \varepsilon_0 |r_i - r_j|^3} \left[ \frac{d\dot{l}_i}{dt} \frac{d\dot{l}_j}{dt} \right]$$

where $q_i$ is the charge of the dipole associated with each nanofibril, $r_i$ is the stationary position of the $i^{th}$ nanofibril’s open end and $\frac{d\dot{l}_i}{dt}$ is a unit vector perpendicular to $\dot{d}l_i$. The correction coefficient $c_{hyd}$ behind the first term of (12) takes into account the hydrodynamic loading of water around the beam and is simply given as [75],

$$c_{hyd}^y = 1 + \frac{\pi \rho_{water}}{4 \rho_{beam}}$$

Applying the Lagrange equation [73],

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{y}_i} \right) - \frac{\partial L}{\partial y_i} = F_i^d + F_i^s \quad i = 1, 2, 3, ..., N$$

We will end up having $N$ independent equations. Here, $F_i^d$ and $F_i^s$ account for the damping force (cantilever beam vibration in water as a viscous medium) and other external non-conservative forces, respectively. By solving the abovementioned $N$ equations for the steady state condition, one can obtain all the possible resonant frequencies and amplitudes of oscillation of the nanofibrils in the medium. These equations in the frequency domain can be re-arranged in the form of a generalized eigenvalue-eigenfunction problem,

$$\left( -\omega^2 M + i\omega F_d + K \right) \vec{F} = \vec{F}_0$$

where $\omega$ is the natural resonant frequency of the system, and $Y$ is an $N \times 1$ vector representing the amplitude of oscillation of the fibrils at that frequency. The index 1 on the right-hand side (excitation vector) corresponds to one initially-disturbed nanofibril. Defining $Q_i$ as the quality factor for the vibration of the $i^{th}$ nanofibril in water, and $s_i$ and $m_i$ as,

$$s_i = \frac{1}{2} E_i \left( \frac{\pi}{2E_s} \right)^2 l_i, \quad m_i = c_{hyd}^y \rho_i A_i \left( \frac{3\pi}{2\pi} \right) l_i$$

The $N \times N$ matrices $\vec{K}$ (equivalent spring constant), $\vec{M}$ (equivalent mass), and $\vec{F}_d$ (equivalent damping) [76] in (16), can be written as,

**TABLE 1. THE POSSIBLE NATURAL RESONANT MODES AND CORRESPONDING FREQUENCY RANGE IN BIFILMS RESPONSIBLE FOR POTENTIAL EM SIGNALING.**

| Schematic | Frequency Range |
|-----------|-----------------|
| Cantilever beam Mode | $\sim$20 kHz-600 MHz |
| Longitudinal Spring Mode | $\sim$0.2GHz-6GHz |
| Transverse Spring Mode | $\sim$10GHz-50GHz |
| Combined Fibril+Cell Mode | $\sim$0.5GHz-5GHz |
As can be seen, the non-diagonal elements of the matrix $\mathbf{K}$ represent the electromagnetic coupling between the nanofibrils. These non-diagonal elements are in fact representing the communication among adjacent nanofibrils. As will be discussed later, the ratio of non-diagonal elements to the diagonal elements ($\kappa_i/s_i$) is critical in establishing synchronized vibration among nanofibrils. By synchronization, we just mean that the amplitude level of nanofibrils displacement are a noticeable fraction of the oscillation amplitude of that initially disturbed nanofibril. All the possible resonant frequencies of the system (frequencies of EM-based communication) are the solution of following equation,

$$\mathbf{\overline{K}} - \omega^2\mathbf{\overline{M}} + i\omega \mathbf{\overline{F}}_d = 0$$  \hspace{1cm} (19)

The corresponding amplitude of oscillation for all the nanofibrils associated at each eigenfrequency ($\omega_i = \text{Re} \{\omega_i\}$) is also given by,

$$\mathbf{\overline{\psi}_i} = (\mathbf{\overline{K}} - \omega^2\mathbf{\overline{M}} + i\omega \mathbf{\overline{F}}_d)^{-1} \mathbf{\overline{F}}_0$$  \hspace{1cm} (20)

The more non-zero elements the vector $\mathbf{\overline{\psi}_i}$ contains, the stronger is synchronization among the cells at that frequency which is determined by the strength of $\kappa_i/s_i$.

For simple demonstration of the concept and capability of our proposed approach, we have generated 2000 non-intersecting nanofibrils using a packing algorithm [77]. The nanofibrils are generated such that they are all confined within a box with dimensions $8 \times 8 \times 4 \ \mu$m$^3$ (~0.3% volume fraction) to represent a biofilm sample. Nanofibrils length distribution is considered to be uniform, $L\sim U(0.1, 6) \ \mu$m. Using those previously used values of the mass density ($\rho$), cross section ($A$) and bending rigidity ($EI$), and setting nanofibrils dipole charges [29] $q=5e$ ($e$ is the electron charge value), (19) and (20) are solved for the resonant frequency (communication frequency) as well as the vibration amplitude of all nanofibrils in response to one initially-disturbed nanofibril. The quality factor for a cantilever beam vibrating in water (biofilm background medium) is set to be $Q\sim4$ (see Appendix B). Fig. 13(a) illustrates the resulted frequency spectrum. As can be seen, based on the cantilever beam vibrational mode, $S$ aureus cells that are used in this simulation can potentially use electromagnetic signals within the kHz-MHz range. This potential spectrum depends on the modeling parameters and is not unique. As there are many uncertainties in experimental values for these parameters, the spectrum can slightly shift up or down. Also it is noted that in this simulation, we have only considered the fundamental mode. Considering higher order modes of cantilever beam, frequency spectrum also shifts upward. The relative amplitude of oscillation of nanofibrils at two of the fundamental mode’s resonant frequencies 13.6 kHz, and 3.3 kHz are calculated and shown in Fig. 13(b), and Fig. 13(c), respectively. Here, all the amplitudes are normalized to the amplitude of the nanofibril having maximum oscillation level. It is obvious that in response to the initial vibration of one nanofibril, other nanofibrils start vibrating by the transferred electromagnetic signal. The synchronized motion with large amplitudes happens only at subset of all possible resonant frequencies. It should be noted that the level of synchronization decreases as the resonant frequency increases. This is due to the fact that the cantilever beams vibrating at higher frequencies are stiffer and the EM field is not strong enough to exert force on the nanofibrils. Since there are uncertainties on the reported values for the nanofibrils dipole moment (charges), another simulation considering stronger dipole charges $(q=15e)$ is carried out and the result is shown in Fig. 14(a), Fig. 14(b), and Fig. 14(c) depict the relative amplitudes of vibration at 8 kHz and 27.6 kHz, respectively. It is shown that stronger dipole moment enhances the electromagnetic coupling which in turn will increase the synchronization between the nanofibrils. Additionally, as the electromagnetic force becomes stronger, the resonant frequencies with high synchronization level potentially shift upward. The impact of quality factor on the synchronization and frequency spectrum was also investigated by considering, for instance a lower quality factor value ($Q=2$) for the nanofibrils’ vibration. It can be observed from Fig. 15(a) that the frequency spectrum slightly changes and synchronization level becomes smaller when the loss increases. This is somehow expected because oscillation amplitude of transmitting nanofibril gets attenuated quickly and then electromagnetic coupling strength reduces.

The same procedure was applied to study the spring vibrational mode [78] illustrated in Fig. 7(c). The Young modulus for the spring mode is set to be 25 GPa [25]. Considering spring modes, the spectrum shifts to the gigahertz frequencies as shown in Fig. 16(a), mainly because of larger stiffness compared to the cantilever mode. Because of this stiffness, nanofibrils cannot excite each other to have synchronization (Fig. 16(b), and Fig. 16(c)).

**APPENDIX B**

From this study, one would be able to unravel the damped behavior of nanofibrils vibration as they are immersed in water background of biofilm (viscous background) and then find corresponding quality factor, $Q$. In order to find the $Q$ factor, COMSOL Multiphysics is utilized in this section considering both cantilever beam and spring modes. Fig. 17(a), and Fig. 17(b) illustrate two different scenarios where an amyloid nanofibril is once attached to a cell membrane (cantilever beam mode) and once is suspended...
within the biofilm individually (spring mode), respectively. The cell is assumed to be spherical (\(R = 440 \text{ nm}\)) and the nanofibril is modeled as a solid beam with 1 \(\mu\text{m}\) length having bending rigidity \(EI = 0.8 \times 10^{-26} \text{ N.m}^2\) (for the cantilever beam mode) and having Young modulus \(E = 25 \text{ GPa}\) (for the spring mode). Water background is assigned to the simulations with dynamic viscosity 1.02 mPa.s. An external force with duration \(T_0\) is applied to the nanofibril’s open-end(s) in time-domain. The motion of the nanofibril is

![Figure 13](image)

FIGURE 13. (a) Possible resonant frequencies of electromagnetically-coupled amyloid fibrils (cantilever beam mode, \(Q = 23\)). (b) Relative amplitude of vibration of fibrils at one of those eigenfrequencies (3.3 \(k\text{Hz}\)). (c) Relative amplitude of oscillation of fibrils at 3.3 \(k\text{Hz}\).

![Figure 14](image)

FIGURE 14. Impact of stronger dipole moment (\(q = 15 e^-\), \(Q = 3\)) on the synchronization and natural resonant frequencies. (a) The resulting frequency spectrum. (b) The relative amplitude of fibrils’ vibration is plotted at 3 \(k\text{Hz}\). (c) The relative amplitude of fibrils’ vibration is plotted at 27.5 \(k\text{Hz}\).

![Figure 15](image)

FIGURE 15. Impact of lower quality factor (\(Q = 2\)) on the synchronization and natural resonant frequencies. (a) The resulting frequency spectrum. (b) The relative amplitude of fibrils’ vibration is plotted at 3 \(k\text{Hz}\). (c) The relative amplitude of fibrils’ vibration is plotted at 13.7 \(k\text{Hz}\).

![Figure 16](image)

FIGURE 16. (a) Possible resonant frequencies for the spring mode. (b) Relative amplitude of fibrils’ oscillation for spring mode at 0.5 \(k\text{Hz}\). (c) Relative amplitude of fibrils oscillation for spring mode at 5.13 \(k\text{Hz}\). Only the initially-excited fibril vibrates and cannot couple to other fibrils.
then monitored. The duration of applied pulse ($T_0$) is 3 µs and 0.5 ns for the cantilever beam mode and the spring mode, respectively. In fact, $T_0$ is inversely close to the resonant frequency of motion for each mode ($\sim$180 kHz, and $\sim$1 GHz, respectively). Fig. 18(a), and Fig. 18(b), show the time-domain profile of nanofibril’s open-ends vibration for cantilever beam and spring mode, respectively. The results are also provided assuming free-space background instead of water. From this figure, the damping effect can be readily captured. The peak of damped vibration can be written as,

$$d_{\text{peak}} = \pm d_0 e^{-\frac{\pi f_0}{Q}}$$

Where $f_0$ is the frequency of vibration and $Q$ is the quality factor. Using the information in this figure, the quality factor associated with the cantilever beam mode and the spring mode are found to be 4 and 2.5, respectively. Based on this figure, nanofibrils experience more than at least two cycles indicating that oscillation is not over-damped and resonance sustains well in the system.

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