SIMULATION OF INTERACTION BETWEEN BACILLUS SUBTILIS BACTERIA AND SILICON SURFACE

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Abstract – The investigation of the physical and energy affinity between *Bacillus Subtilis* bacterial cell wall and the silicon surface is discussed in the frame of finding optimal conditions for efficient immobilization of bacteria in porous silicon.

I. INTRODUCTION

The high chemical toxicity of pesticides is strong stated fact. Now it is the main ecologic problem in the world. Consequently, it is needed to create safe and effective biological products for plant diseases struggle. Biopesticides, in contrast to chemical pesticides, are generally characterized by high selectivity of action against harmful organisms and by lower non-target kinds toxicity. Endophytic bacteria are used as the base of such biopesticides. They penetrate into the inner plant tissues and prevent the ingress of pathogens diseases into the plant organisms. Next problem is the immobilization of the bacteria in special “containers”, for example, in pores of porous materials. We investigate the possibility of the above problem solution in the frame of molecular dynamics methodology.

II. OBJECTS OF INVESTIGATION

In this work we investigate the possibility of use a porous material (porous silicon as wide known material in microelectronics), which is the biologically active material at the expense of increased chemical reactivity, as a container for the Bacillus Subtilis bacteria. Bacteria, located in the pore, is isolated from external influence, i. e., it is "preserved" and its fermentation processes are slowed, which will extend the term of the storage and simplify transportation conditions. The problem is to determine the physical and energy affinity between Bacillus Subtilis bacterial cell wall and the silicon surface in order to find optimal conditions for efficient immobilization of bacteria in porous silicon.

Bacterial protoplast is surrounded by peptidoglycan, which is essentially one giant molecule, "crosslinked" through glycosidic and peptide bonds, and composing the bulk of the cell wall of Gram-positive bacteria, which include the Bacillus Subtilis bacteria.

Thus, investigation objects are the fragment of Baillus Subtilis bacterial cell wall (single-layer system of peptidoglycan molecules (Fig. 1 and 2)) and the surface of silicon with the main crystallographic orientations <110> and <001> [1, 2, 3]. Silicon with crystallographic orientation <111> is not considered in this research, because this orientation is not peculiar to the pores of silica. Since the a typical pore of silicon size order of several microns, and the size of the cell wall fragments order of tens of nanometers, it is possible to neglected the curvature of the pore walls.

III. METHODOLOGY

Modeling the interaction between single-layer system of peptidoglycan molecules and silicon surface performed using HyperChem software package intended for the quantum-mechanical (first-principles) and molecular-dynamic simulations of atomic structures. Force fields used by HyperChem are MM+ (based on the MM2), Amber, OPLS and BIO+ (based on the CHARMM) [4]. The simulated murein layer is a 16 repeating peptidoglycan molecules that linked together by peptide bridges, as shown in Fig. 2. Obtained structure of murein is shown in Fig. 3. The spatial optimization of the murein structure with a view to minimize the potential energy performed using a force field Mm+ and spatial optimization algorithm of Polak-Ribiere [5]. The minimum total energy of a single-layer murein molecule is about 325 kcal/mol with a standard deviation equal to 0.01 kcal/mol.

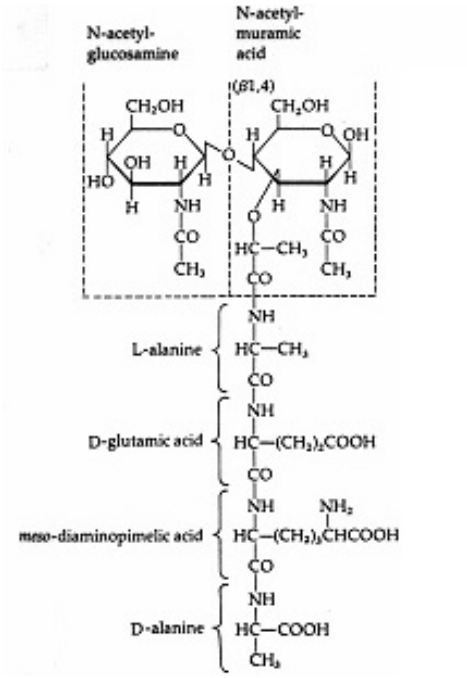

Figure 1 – The structure of the repeating peptidoglycan molecules

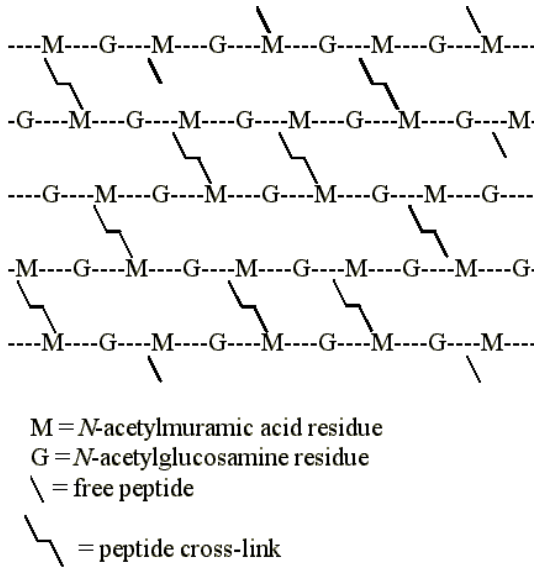

Figure 2 – The single-layer system of peptidoglycan molecules

IV. RESULTS AND DISCUSSION

Simulation results of the interaction between obtained murein layer and the surface of silicon with the crystallographic orientation <110> showed that decreasing the distance between the silicon surface and murein, magnitude of the total potential energy of the murein layer decreases to ~30 kcal/mol (at the distance ~3Å between molecular monolayer system murein and the silicon surface), which indicates a good affinity between murein layer and surface of silicon with this crystallographic orientation. The results of modeling the interaction between murein and the surface of silicon with the crystallographic orientation <001> showed that the total potential energy of the molecule murein decreased to only ~98 kcal/mol, which indicates that the physical and energetic affinity between the murein layer is best possible when silicon has crystallographic orientation <110>.

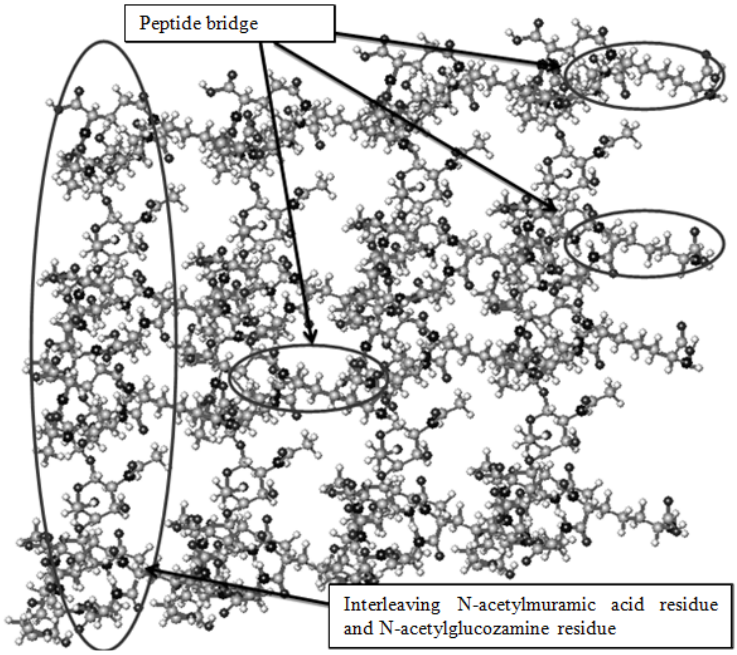

Figure 3 – Single layer of peptidoglycan molecules

V. Conclusion

Thus, the results of investigation presented in this paper showed: the possibility of using porous silicon as a container for transportation and storage of Gram-positive bacteria such as Bacillus Subtilis bacteria; an effective method for solving such problems is the method of molecular dynamics; the surface of silicon with crystallographic orientation <110> is the best affinity to single-layer of peptydoglican molecules, which is the cell wall of Gram-positive bacteria.

Acknowledgments

This work was carried out under the Project No 11-1080B "To develop and adapt to the conditions of industrial production methodology parameter optimization of the fermentation process of obtaining Betaprotektin biopesticide based on mathematical modeling and investigate the immobilization of microbial cells using nanostructured materials".

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