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IMPACT OF DISORDER AND MANUFACTURING COST ON THE EFFICACY OF MECHANO-BACTERICIDAL NANOSTRUCTURES

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Abstract

This work presents a combined mathematical and simulation modeling approach to evaluating the mechano-bactericidal effect of nanostructured surfaces. We show for the first time that a mathematical expression of mechanical stress can be derived from bacterial and nanopillar properties. By applying the model in simulations, we demonstrate that the nanopillar design can be optimized to achieve higher bacteria-killing efficiency. We also show that those high-end fabricating techniques only moderately improve antibacterial efficiency at much higher cost. The study validates the mechano-bactericidal concept, provides a quantitative model for stress, and offers insights for optimizing nanostructure design.

Keyword: *Mechano-bactericidal, Nanopillar, Bacteria*

1. Introduction

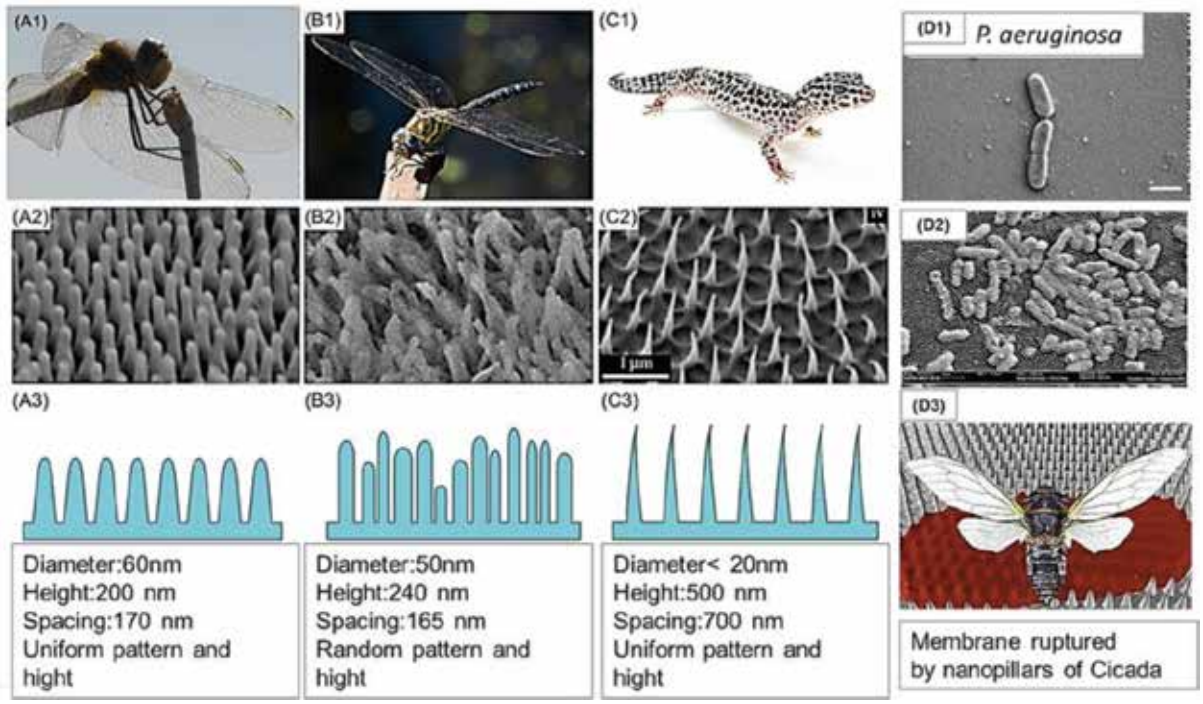
Bacterial contamination and resulting infections present a serious danger across various environments, including hospitals, the food industry, and community settings. Antibiotics are the most common treatment for bacterial infections. However, antibiotics have led to the development of bacterial resistance, making routine treatment of bacterial infections increasingly difficult. Eliminating bacteria effectively without causing bacterial resistance has become an important research topic today.

In the past decade, the use of mechano-bactericidal nanostructured surfaces has emerged as a potential alternative (Linklater 2021, Li 2021, Agbe 2024). Researchers found that the physico-mechanical interactions between such nanostructured surfaces and bacteria lead to bacterial killing or prevention of bacterial attachment, and thus are promising in circumventing bacterial infections.

This approach is inspired by nature. Researchers have found that the surfaces of cicada and dragonfly wings exhibit antibacterial properties due to their unique nanoscale pillar structure (Ivanova 2020, SHT 2013). Details of such a nanoscale pillar structure are shown in Fig. 1 (Dickson 2015). Com-

pared to bacteria incubated on flat surfaces, bacteria attached to nanopillared surfaces appeared deflated or elongated, as the pillar structure induces mechanical stress on the bacterial cell membrane. When the stress exceeds the cell membrane's elasticity, the membrane ruptures, and the bacteria die.

Figure 1. *Illustration of mechano-bactericidal surfaces in nature ((Dickson 2015)*

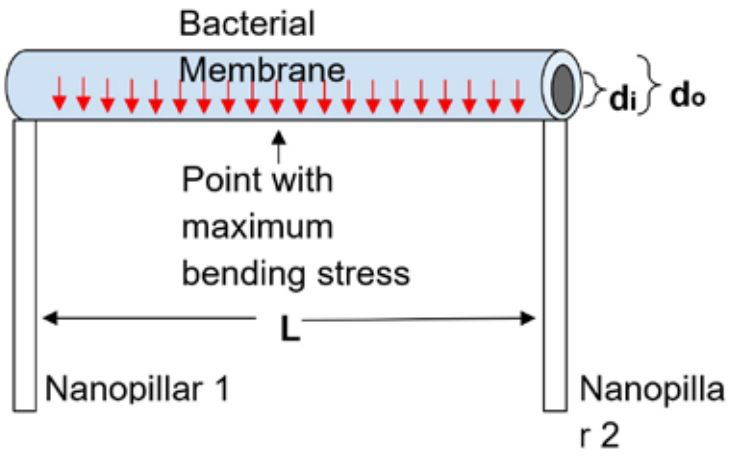


In this paper, we use both mathematical and simulation modeling to study the mechanical stress imposed by nanopillared surfaces on bacteria. We show for the first time that a mathematical expression of mechanical stress can be derived from bacterial and nanopillar properties. By applying this model in simulations, we demonstrate that the nanopillar design can be optimized to achieve the highest bacteria-killing efficiency. Furthermore, we compare the antibacterial efficiency of modern high-end and low-end nanoscale fabricating techniques, and show that those high-cost techniques provide only a moderate improvement in antibacterial efficiency.

2. Research Method

2.1 Mathematical Modeling

Figure 2. *A bacterial membrane falls onto two nanopillars*



To evaluate how nanopillars kill bacteria attached to them, we use a mechanical engineering approach to derive the bending stress imposed by the weight of a bacterial membrane on a nanopillar surface. When the bending stress exceeds the membrane's stress threshold, the membrane is considered killed.

The shape of a bacterium can be approximated as a spherocylinder, i.e., a circular tube. We use d_o and d_i to represent its outside and inside diameters, respectively. Therefore, the tube thickness is $t = \frac{d_o - d_i}{2}$. Normally, the member length is much larger than its diameter. When placed on a nanosurface with densely packed nanopillars, a membrane could land on multiple nanopillars. Between two adjacent nanopillars, as shown in Fig. 1, the membrane segment is modeled as a beam (Wikipedia 2025) in the mechanical engineering sense, supported at its ends. Due to the membrane's uniform weight distribution, it will experience bending stress along its trunk between the two supporting pillars. Clearly, the maximum bending stress occurs midway between the two pillars. Following the Euler-Bernoulli beam theory (Wikipedia 2025), such maximum bending stress is

$$\sigma_{max} = \frac{M \cdot y}{I_c}$$

Where M is the bending moment, y is the distance from the beam's neutral axis to the middle point along the dimension of the circular tube, and I_c is the centroidal moment of inertia of the beam's cross section, which is a circular tube. These two parameters, in this particular scenario of simply supported beams with uniformly distributed load, can be calculated according to (Wikipedia 2025):

$M = \frac{wL^2}{8}$ (w is the uniform weight per length unit of the membrane)

$$y = \frac{d_o - d_i}{4}$$

$$I_c = \frac{\pi}{64}(d_o^4 - d_i^4)$$

So

$$\sigma_{max} = \frac{\left(wL^2/8\right)\left(d_o - d_i\right)/4}{\left(\pi/64\right)(d_o^4 - d_i^4)} = \\ = \frac{2wL^2}{\pi(d_o^2 + d_i^2)(d_o + d_i)} \quad (1)$$

We assume $\sigma_{critical}$ is the bending stress threshold for a given bacterial type. When $\sigma_{max} \geq \sigma_{critical}$, the bacteria are considered killed. Note that while w, d_o, d_i and $\sigma_{critical}$ are all bacterial characteristics, L is the pillar-to-pillar spacing and determined by the nanosurface design.

The above mathematical model is the foundation of our analysis. Equation 1 indicates that when a bacterium is placed on a nanostructured surface, its membrane may fold onto nanopillars, resulting in high membrane stress and killing the bacterium. On the other hand, if nanopillars are too sparse, the chance of a bacterium falling onto them is low, thus a lower chance of breaking. Therefore, it is intriguing to further analyze how nanostructured surfaces impact antibacterial effectiveness.

2.2 Simulation

A computer-based simulation is conducted to further model how nanostructured surface design affects antimicrobial killing efficiency. The simulation models both nanostructured surfaces and bacteria.

A grid is generated to simulate a nanostructured surface with pillars. Each point in the grid represents a pillar location. The point lies within a circular area of the same diameter as the pillar. The distance between neighboring grid points is the pillar-to-pillar spacing. There are many bacterial types with different geometries and sizes. *E. coli* is a commonly studied bacterial type and is used in the simulation.

All the properties of the nanostructured surface and bacterium are listed in Table 1 below.

In the simulation, 1000 bacterial samples are generated with a specified size distribution and a specified location on the grid. The location of a bacterial sample is determined by two randomized parameters: the centroid and the orientation. Once a bacterium is generated, it needs to be decided on how it interacts with the pillars. To this end, the grid and bacterial locations are used to determine

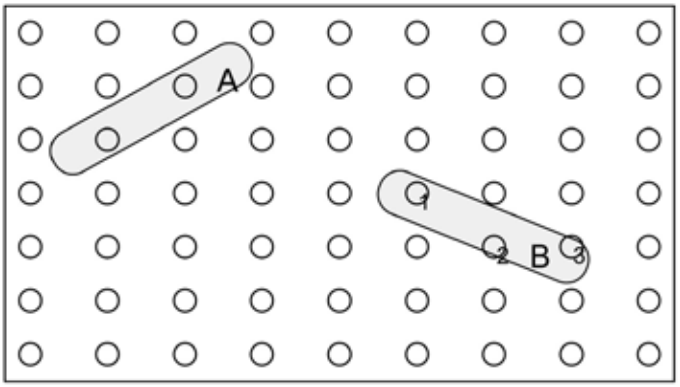
how many, if any, pillars support the bacteria (i.e., overlap with the bacteria). When deciding whether a pillar supports a bacterium, the pillar's diameter is taken into account. As long as any of the circular area of a pillar overlaps with a bacterium, the pillar is considered to support the bacterium.

Table 1. *Properties of the bacteria and the nanostructured surface used in the simulation*

	Property	Variable	Typical Values
Bacterium (*E. coli)*	Length	s	3000 nm
	Weight on unit length	w	10^{-12} gram per μm
	Outside diameter	d_o	500 nm
	Inside diameter	d_i	490 nm
	Thickness	$(d_o - d_i)/2$	5 nm
	Critical bending stress	$\sigma_{critical}$	Take a fixed value in the simulation
Nanostructured surface	Pillar diameter	d_p	36 nm [6]
	Pillar-to-pillar spacing	L	1000 nm

Fig. 3 shows two bacteria, A and B, placed on a grid. Because Bacteria A is supported by exactly 2 pillars, its σ_{max} calculation is straightforward. For Bacteria B, 3 pillars support it. In this case, the 3 pillars are first sorted along the length dimension of the bacteria. Next, the neighboring bacterial pairs with the longest distance are found, and that distance is used to calculate σ_{max}. For example, in Fig. 3, the distance between Pillars 1 and 2 is longer than that between Pillars 2 and 3. Therefore, Pillars 1 and 2 are used to calculate the force imposed on the bacterium.

Figure 3. *Simulated nano pillar array and two randomly placed bacteria*



$\sigma_{critical}$ is a bacteria-specific threshold. It's difficult to obtain from the real world. In our simulation, we use the settings in Table 1 and run it 1000 times. We then assign $\sigma_{critical}$ the 50% percentile of σ_{max}. In other words, we assume a 50% bacteria-killing rate is the baseline when the nanostructured surface uses the common settings in Table 1. We believe this doesn't affect our study, as we are more interested in the relative impact of varying surface design parameters.

3 Results Analysis

3.1 Impact of Nanostructure Geometry

The first simulation assesses how pillar geometry impacts antibacterial efficiency. Two types of pillar geometry are evaluated: pillar-to-pillar spacing and pillar diameter. As shown in Fig. 4, the optimal pillar-to-pillar spacing is neither too large nor too small relative to the bacteria's size. The insight is that when it is too small, a bacterium has

a high chance of falling onto multiple pillars, thereby reducing the inter-pillar distance and lower stress. When the distance between the nanopillars increases, the stress increases, thereafter the bacterium membrane has a high chance to break.

It is worth noting that a previous experiment (Dickson 2015) showed that smaller, more closely spaced pillars are more effective at killing bacteria. Our analysis indicates that the optimal pillar-to-pillar spacing lies between too large and too small. It is essentially relative to the bacterial size.

Figure 4. *Effect of pillar-to-pillar spacing on bacteria killing efficiency*

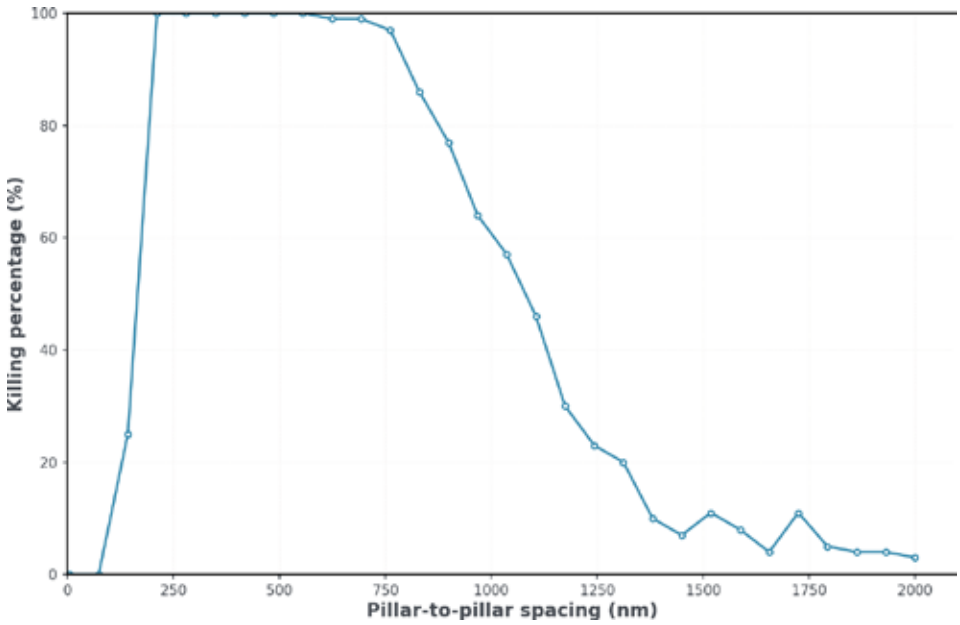
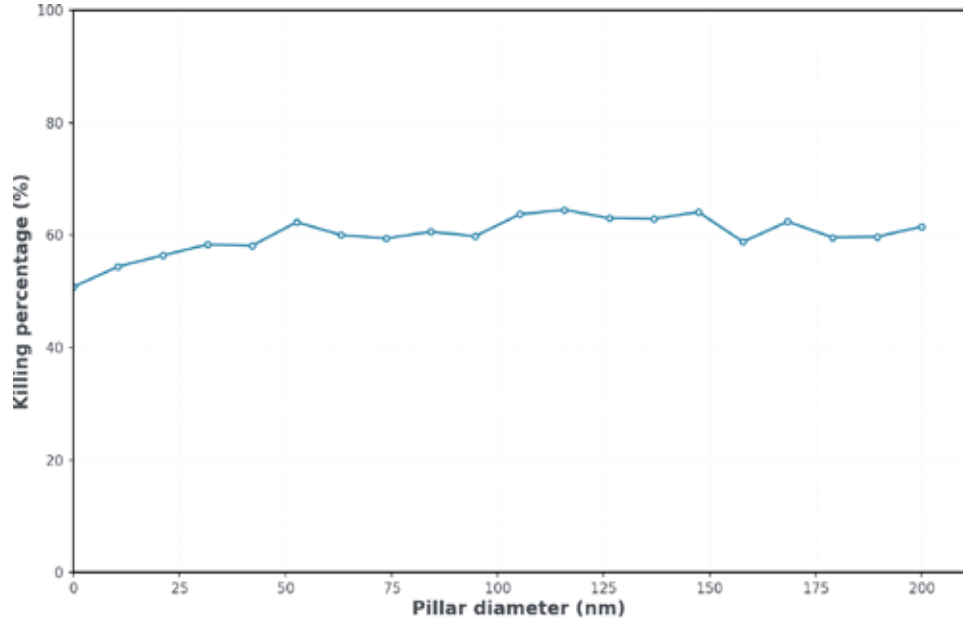


Fig. 5 shows another simulation run where the pillar diameter increases from 0 to 200 nm. The bacteria-killing efficiency has a mild increase. The insight is that when the pillar diameter is larger, the chance of a bacteria falling onto pillars is higher, as the bacteria also have a diameter. This benefits the killing efficiency. Nevertheless, the importance of pillar diameter is much less than pillar-to-pillar spacing.

Figure 5. *Effect of pillar diameter on bacteria killing efficiency*



In another two simulation runs, we vary the bacteria size while keeping the pillar design unchanged. The two bacterial sizes are Bacteria Outside Diameter (d_o) and Bacteria Length (s). As shown in Figs. 6 and 7, increasing bacteria size improves bacteria killing efficiency. The insight is that larger bacteria have a higher chance of falling onto nanopillars.

Figure 6. *Effect of Bacteria Outside Diameter on Bacteria Killing Efficiency*

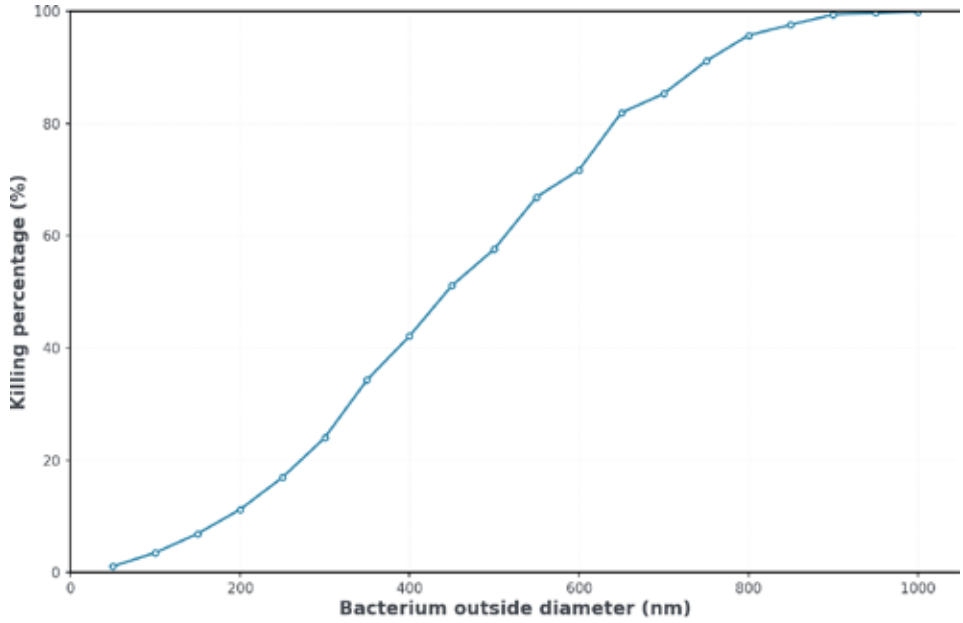
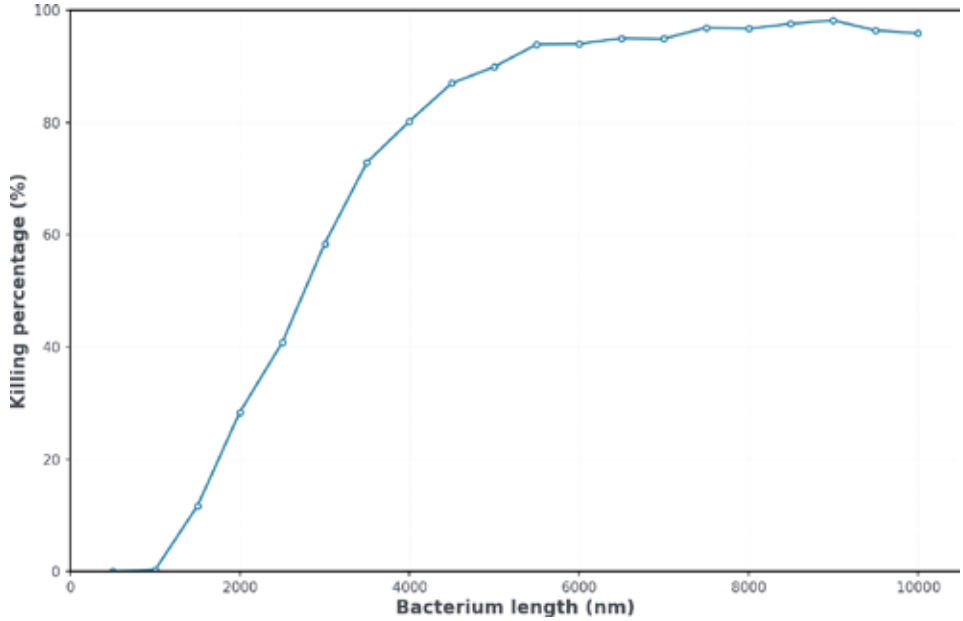


Figure 7. *Effect of Bacteria Length on Bacteria Killing Efficiency*



3.2 Impact of Disorder and Manufacturing Cost

In previous simulations, the nanostructure is assumed in perfect order, i.e, each pillar position is precise, and all pillars exist. In reality, nanostructure is fabricated by expensive machines. Due to fabrication errors, the nanostructure could be imperfect. For example, there are three popular techniques in the industry for fabricating nanostructures: E-beam Lithography (Zhu 2024), Nanoimprint Lithography (NIL) (Dhull 2024), and Self-Assembly Method. They have different levels of cost and fabrication quality, as shown in Table 2.

Table 2. *Three popular nanostructure fabricating techniques*

Fabricating Technique	Disorder Level	Non-Uniformity	Defect Density	Cost
E-beam Lithography	Very Low	< 5 nm	< 0.1 defects/μm²	High
Nanoimprint Lithography (NIL)	Moderate	5–15 nm	0.5–5 defects/ μm²	Moderate
Self-Assembly Method	High	20–50 nm	> 10 defects/μm²	Low

As Table 2 shows, every fabricating technique introduces errors: either the pillars are displaced, not uniformly distributed, or in defect. In this section, we simulate how an imperfect nanostructure affects the bacteria-killing efficiency. Three types of errors are considered in the simulation:

Pillar Dislocation: A pillar is dislocated from its original location. This is modeled by introducing a Gaussian noise to the pillar location. The standard deviation of the Gaussian noise is used to control the magnitude of the Pillar Dislocation

Defect Density: A pillar has a defect. This is modeled by introducing Defect Density that describes statistically, on average, how many pillars in an area have defects, thus not being fabricated

Regional Defect Percentage: An entire region of pillars has defects. This is modeled by dividing the entire pillar array into 10×10 regions, and each region has a probability that all the pillars within are not fabricated. This probability is called the Regional Defect Percentage.

Figures 8–10 show that increasing any of the three error types decreases the bacteria-killing efficiency. Nevertheless, we observe that within the error range of the three fabricating techniques in Table 2, the bacteria-killing efficiency does not appear to differ significantly. For example, Defect Density is the most clearly defined error type in Table 2. As shown in Fig. 9, the bacteria-killing efficiency only decreases from 60% to 50% when switching from E-beam Lithography, the most expensive fabrication technique, to the Self-Assembly Method, the least expensive one. This observation suggests that low-cost fabrication techniques may be preferred when mechanical stress is the primary anti-bacterial factor.

We have also simulated the scenario with multiple error types. As shown in Fig. 11, both Pillar Dislocation and Defect Density. The figure shows that multiple error types have compound effects: when the magnitudes of both error types increase, the bacteria-killing efficiency decreases more significantly than when only one error type increases.

Figure 8. *Effect of pillar displacement on bacteria killing efficiency*

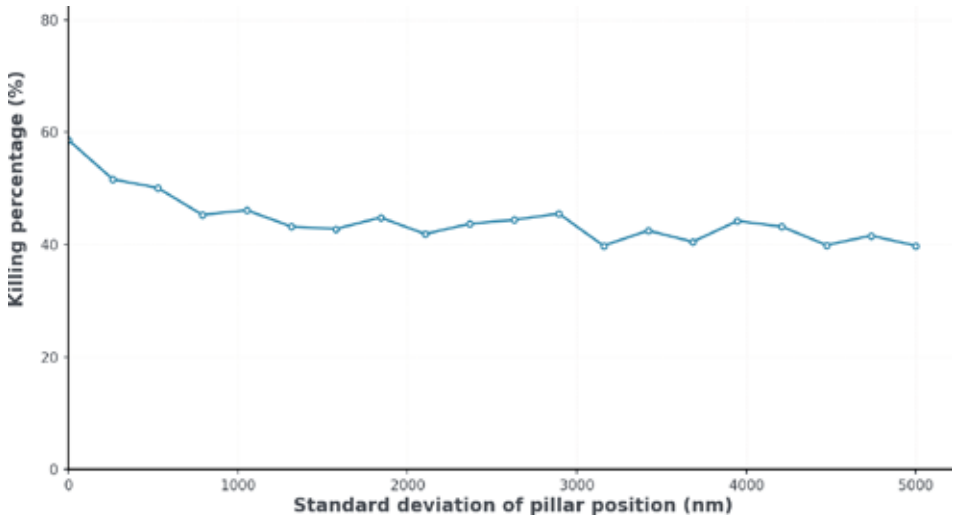


Figure 9. *Effect of individual pillar defect on bacteria killing efficiency*

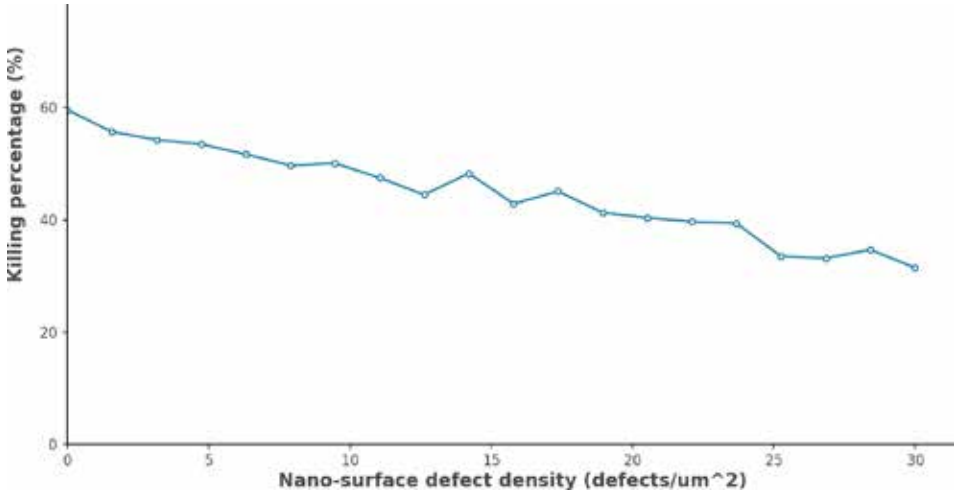


Figure 10. *Effect of a block of pillar defect on bacteria killing efficiency*

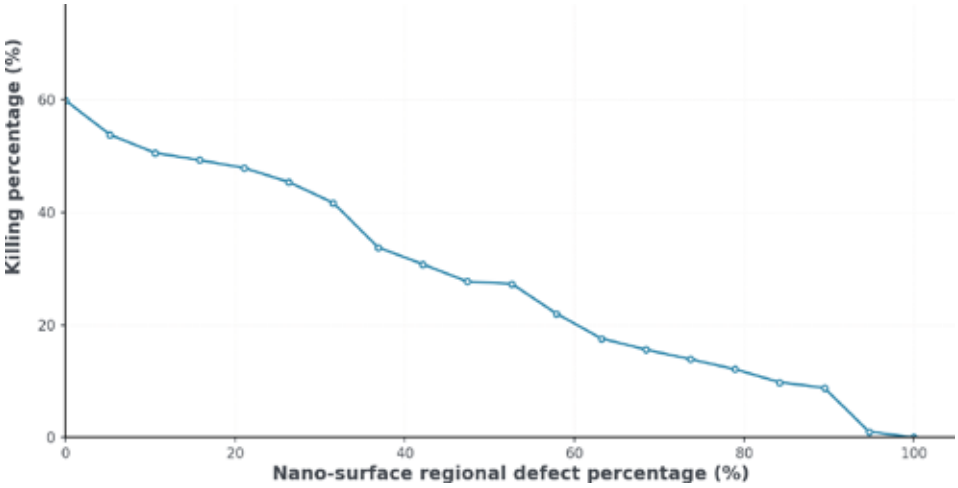
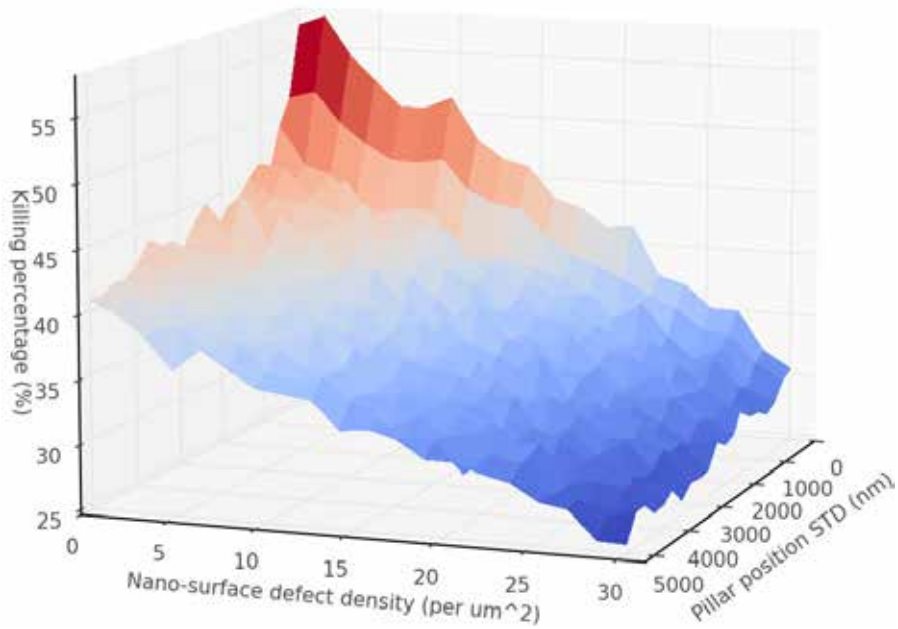


Figure 11. *Effect of co-existence of pillar dislocation and defect on bacteria killing efficiency*



Conclusion

This study proposes both a mathematical and a simulation model to explain the effectiveness of nanopillared surfaces in killing bacteria. We use a mechanical engineering approach to derive an analytical expression of the maximum stress imposed by nanopillars on bacterial membranes. The stress is compared to a critical stress threshold to determine whether the bacteria are killed by nanopillars. We further develop a simulation model to evaluate the interaction between bacteria and nanopillars. The results show that the pillar distribution and size must fall within a specific range to optimize the bacteria-killing efficiency. We further evaluate how existing nanoscale fabrication techniques, with varying costs and quality levels, affect antibacterial effectiveness. The results show that although higher-end fabricating techniques yield higher bacterial-killing efficiency, the gain is marginal compared to most cost-effective fabricating techniques.

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