Compressive Behaviors of Micropillar Patterns Made of PDMS Material using the Finite Element Method

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Abstract. Hydrophobic surface is a surface having the ability of water repellent which is frequently coated on medical devices and marine structures. This hydrophobic surface can fabricate from micro-pattern sheets consisting of groups of micropillars arranged into unique micro-patterns which are normally made of low surface energy materials. Thai Microelectronics Center (TMEC) has fabricated micropillar sheets from PDMS for various micropillar array patterns from soft lithography techniques. However, these micropillar sheets were relatively weak under pushing forces. This research aimed to understand compressive behaviors of rectangular prism micropillars having different aspect ratios (ratio of width to length of a rectangular cross-section) and micro-patterns consisting of micropillars having rectangular cross-section and square cross-section by using ANSYS Mechanical APDL program. We found that the aspect ratio of prism micropillars had not influences on both elastic stiffness and compressive strength under compressive loading. The lateral collapse of micropillars were observed on all micro-patterns during compressive loading. Furthermore, the sharklet micro-pattern had the highest compressive strength with maximum compressive pressure of 9.87 kPa. Finally, as loading contact area of micropatterns increases, the compressive strength increases while the water contact angle decreases.

Keywords: Hydrophobic surface, polydimethylsiloxane, micro-pattern, finite element analysis, ANSYS.
1. Introduction

Biofouling on surfaces, such as virus, bacteria, and disease on medical equipment surface and food applications have been a health risk. Moreover, biofouling of seaweed, bacteria and barnacles on marine engineering structures and tools have been a significant impact on structural damage [1]. To prevent biofouling on these surfaces, superhydrophobic films are often coated on medical equipment or marine engineering structures. Polydimethylsiloxane (PDMS) materials are generally used to fabricate superhydrophobic surfaces because of their low surface energy, non-toxic, non-flammable and good biocompatibility [2]. The hydrophobic properties are regulated by the water wetting angle of the surface. Gomes, Souza and Silva [3] classified the wettability property of surfaces by a water contact angle. Firstly, if the water contact angle is under 90 degrees, it is called a hydrophilic surface. Secondly, if the water contact angle is between 90 to 150 degrees, it is called a hydrophobic surface. Thirdly, if the water contact angle is greater than 150 degrees, it is called a superhydrophobic surface. This surface can improve hydrophobicity by creating rough surface consisting of micro- or nano-structures on substrate surfaces [4]. The rough surface can be prepared from cultivating micropillars on the substrate surfaces; however, micropillars could experience self-mating micropillars upon the pushing force. As result, hydrophobic properties would blunder away [5]. Microstructure can be robust if micropillars are designed with unique sizes and shapes. For this reason, many researches have focused studies not only on micro- and nano-patterns which prevent biofouling but also on mechanical behaviors of hydrophobic surfaces under various loading conditions. Graham and Cady [6] found that the sharklet pattern on hydrophobic surface could prevent biofouling. Rahmawan et al. [7] fabricated the PUA cylinder-shaped micropillars with silica particles on top of micropillar’s head and compared their shear adhesion strength to non-silica particles. The authors found that the micropillars with silica particles showed higher shear adhesion strength than micropillars without particles. Atthi et al. [8] studied effects of various asperity shapes on superhydrophobic surfaces. The authors found that the pentagonal pillars with square and hexagonal arrays had highest water contact angle of 155.9 degrees. Atthi et al. [9] studied effects of various PDMS micro-structures on hydrophobic and antifouling properties. The authors found that the circular rings with eight stripe supporters (C-RESS) pattern illustrated highest durability that can robust to collapse under external loads. Lu et al. [10] studied effects of pattern size on micro-patterns to prevent bacteria adhesion. The authors found that the pattern size significantly reduced bacteria adhesion, when the pattern size was smaller than the bacteria size, the micro-pattern had better capability to prevent bacteria adhesion. Chebolu et al. [11] studied effects of micro-nano scale patterns made of PDMS material on resisting bacteria activity. The authors found that the highest bacteria adhesion was found on a smooth PDMS. Furthermore, the square and circular micropillars illustrated better resistance to bacteria adhesion. Pakawan et al. [12] studied effects of decreasing the substrate thicknesses on mechanical behaviors of PDMS micropillar sheets under compressive loading in ANSYS Mechanical APDL program. The authors found that the compressive strength and the lateral collapse of micropillars depended on substrate thickness. As the substrate thickness decreased, the compressive strength decreased while the elastic stiffness increased. Furthermore, the micropillar sheet without the substrate did not experience lateral collapse under the compressive load. Thanakhun and Puttipitukporn [13] studied structural behaviors of micropillars fabricated from a core made of PUA material coated with a PDMS material and compared their lateral strength under shear loadings in ANSYS Mechanical APDL program. The authors found that the PUA core coated with 100 nm-thick PDMS micropillar illustrated better lateral strength than pure PDMS micropillar. Cheng et al. [14] studied the sensing device using liquid crystal in micropillar arrays for supporting structure. The authors found that liquid crystal thin film supported in the micropillar arrays were robust and withstand to gravitational forces and mechanical shock. Johari and Shyan [15] used the finite element method to study effect of height and diameter of the cylindrical micropillar made of PDMS material under shear forces. The authors found that deformation increases when micropillar height increased and micropillar diameter decreased. Singh et al. [16] studied deformation of taper and tapered-free micropillars under compressive loading using the finite element method. The FE results showed that straight micropillars had more compressive strength than tapered micropillars. Du et al. [17] analysed the reaction forces in micro-pattern with square micropillars made of PDMS material by using finite element method. Their FE results were compared with the experiment data. The FE results of reaction forces correlated well with the experimental data. Oyunbaatar et al. [18] studied contraction forces of PDMS micropillar arrays with and without grooves on the top of micropillar by using the finite element method. The FE results showed that micropillar with grooves had more contraction force than micropillar without grooves. Liu et al. [19] analysed the automated demolding process of PDMS micropillars with aspect ratio of 6 in LS-DYNA program. The authors found that the FE results correlated well with the experimental data and the peel demolding process had not showed a significant effect on the low aspect ratio of micropillars. Xu et al. [20] used the finite element method to study mechanical properties of SU-8 micropillars under both compressive and nanoindentation test in ABAQUAS program. The authors found that Young’s modulus decreased as diameter of micropillar increased. Furthermore, the yield strength increased as diameter of micropillar increased.

This research was extended work of Pakawan et al. [12] which aimed to understand compressive behaviors of rectangular prism micropillars having different aspect ratios (ratio of width to length of a rectangular cross-
2. Theory

The hyperelastic constitutive models are developed to describe a nonlinear stress-strain relationship which expresses abilities of materials to experience large deformation under small loads and to recover their initial shape upon unloading [21]. In this research, the accurate constitutive model of PDMS under compressive loading was the Mooney-Rivlin 5 parameters [12]. The typical strain energy density function \( W \) can be written in terms of the invariants \( \tilde{T}_i \) and stretch ratios \( \lambda_i \). The invariants can be written as

\[
\tilde{T}_1 = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 \tag{1}
\]
\[
\tilde{T}_2 = \lambda_1^2 \lambda_2^2 + \lambda_2^2 \lambda_3^2 + \lambda_3^2 \lambda_1^2 \tag{2}
\]
\[
\tilde{T}_3 = \lambda_1^4 \lambda_2^4 \lambda_3^4 \tag{3}
\]

The stretch ratio in the \( i \)-direction can be written as

\[
\lambda_i = \frac{L_i}{L_0} = 1 + \epsilon_i \tag{4}
\]

where \( L_0 \), \( L_i \) and \( \epsilon_i \) are the initial length, the instantaneous length and the engineering strain in the \( i \)-direction respectively. The principal stress \( \sigma \) in the \( i \)-direction is derived from the strain energy function as

\[
\sigma_i = \lambda_i \frac{\partial W}{\partial \lambda_i} \tag{5}
\]

2.1 Mooney-Rivlin 5 parameters

The Mooney-Rivlin model is developed from Neo-Hookean model. The strain energy density function of Mooney-Rivlin model depends on the 1st and 2nd invariants and can be written as in Eq. (6).

\[
W = C_{10} (\tilde{T}_1 - 3) + C_{01} (\tilde{T}_2 - 3)
+ C_{20} (\tilde{T}_1 - 3)^2 + C_{11} (\tilde{T}_1 - 3)(\tilde{T}_2 - 3)
+ C_{02} (\tilde{T}_2 - 3)^2 + \frac{1}{D} (J - 1)^2 \tag{6}
\]

where \( W \) is strain energy density function, \( C_{10}, C_{01}, C_{20}, \)
\( C_{11}, \) and \( C_{02} \) are material constants, \( \tilde{T}_1 \) is the 1st invariant, \( \tilde{T}_2 \) is the 2nd invariant, \( D \) is a material incompressibility constant and \( J \) is elastic volumetric ratio.

3. Methodology

Thai Microelectronics Center (TMEC) fabricates micropillar sheets from PDMS material (having ratio of a PDMS monomer to a curing agent ratio of 10:1) for various micropillar array patterns from soft lithography techniques. To study effects of a pillar’s cross section areas on its loading respond, the rectangular prism micropillars having different aspect ratios (ratio of width to length of rectangular cross-sections) as shown in Fig. 1. The micropillar array patterns which consisted of F3, F4, F8 and F13 pattern respectively as shown in Fig. 2-5. These micro-patterns are rectangular prism micropillars (F3 and F13 patterns) and square prism micropillars (F8 pattern). The sharklet pattern is F13. These micro-patterns were modelled in ANSYS Mechanical APDL program. Table 1 illustrates laboratory testing of water contact angles (WCA) of micro-patterns. The hyperelastic material constants acquired from [12].
The FE models of micropillars having different aspect ratios of rectangular cross section areas consisted of 20 µm x 20 µm (ratio of 1:1), 16 µm x 25 µm (ratio of 1:1.56) and 10 µm x 40 µm (ratio of 1:4) as shown in Fig. 6. The FE models were meshed by using SOLID186 elements which were 20-nodes structural solid elements which have 3 translations in the x, y and z directions for each node. The number of elements of each FE models were 4,500, 4,680 and 4,500 elements respectively. Their boundary conditions were that all nodes on the bottom surface were fixed in all degree of freedom while all nodes on the top surface were coupled the displacement in the z-direction. For reducing FE computational time and evaluating convergence of FE results, the replicas of micropillar array patterns were studied. The FE models of F3 pattern consisted of 1, 56, 70 and 84 micropillars respectively as shown in Fig. 7. The FE models of F4 pattern consisted of 1, 56, 70 and 84 micropillars as shown in Fig. 8. The FE models of F8 pattern consisted of 1, 28, 56 and 70 micropillars as shown in Fig. 9. The FE models of F13 pattern consisted of 1, 6, 10 and 12 cells as shown in Fig. 10. Furthermore, all replicas of micropillar array patterns were modeled on 150 µm thick substrate in which the substrate had height and width long enough for focusing only on interactions between micropillars as listed in Table 2-5. The FE models were meshed using SOLID186 elements. The number of elements of each FE models as listed in Table 6-9. The boundary conditions of each FE model were that all nodes on the top surface of micropillars were coupled the displacement in the z-direction while all nodes on bottom surface of the substrate were fixed in all degree of freedom. The surface-to-surface contact without friction was applied to each micropillar. The accurate constitutive model of PDMS was Mooney-Rivlin 5 parameters [12] in which material constants were illustrated in Table 10.
Fig. 7. 3D models of F3 pattern for (a) one micropillar, (b) 56 micropillars, (c) 70 micropillars and (d) 84 micropillars.

Fig. 8. 3D models of F4 pattern for (a) one micropillar, (b) 56 micropillars, (c) 70 micropillars and (d) 84 micropillars.
Fig. 9. 3D models of F8 pattern for (a) one micropillar, (b) 28 micropillars, (c) 56 micropillars and (d) 70 micropillars.

Fig. 10. 3D models of F13 pattern for (a) 1 cell, (b) 6 cells, (c) 10 cells and (d) 12 cells.

Table 1. Water contact angles (WCA) of micro-patterns.

| Micro-patterns | WCA (degree) |
|----------------|--------------|
| F3             | 139.6        |
| F4             | 135.6        |
| F8             | 143.6        |
| F13            | 134.7        |

Table 2. FE models of F3 pattern.

| Number of micropillars | Width (µm) x Height (µm) |
|------------------------|--------------------------|
| 1                      | 700 x 700                |
| 56                     | 1,300 x 1,300            |
| 70                     | 1,300 x 1,300            |
| 84                     | 1,300 x 1,300            |

Table 3. FE models of F4 pattern.

| Number of micropillars | Width (µm) x Height (µm) |
|------------------------|--------------------------|
| 1                      | 1,200 x 1,200            |
| 56                     | 1,200 x 1,200            |
| 70                     | 1,200 x 1,200            |
| 84                     | 1,200 x 1,200            |

Table 4. FE models of F8 pattern.

| Number of micropillars | Width (µm) x Height (µm) |
|------------------------|--------------------------|
| 1                      | 1,500 x 1,500            |
| 28                     | 1,500 x 1,500            |
| 56                     | 2,000 x 2,000            |
| 70                     | 2,000 x 2,000            |

Table 5. FE models of F13 pattern.

| Number of cells | Width (µm) x Height (µm) |
|-----------------|--------------------------|
| 1               | 1,800 x 1,800            |
| 6               | 1,800 x 1,800            |
| 10              | 1,800 x 1,800            |
| 12              | 1,800 x 1,800            |

Table 6. The number of elements of F3 pattern.

| Number of micropillars | Number of elements |
|------------------------|--------------------|
| 1                      | 4,972              |
| 56                     | 28,852             |
| 70                     | 31,948             |
| 84                     | 35,044             |
Table 7. The number of elements of F4 pattern.

| Number of micropillars | Number of elements |
|------------------------|--------------------|
| 1                      | 14,544             |
| 56                     | 179,712            |
| 70                     | 211,104            |
| 84                     | 242,496            |

Table 8. The number of elements of F8 pattern.

| Number of micropillars | Number of elements |
|------------------------|--------------------|
| 1                      | 22,536             |
| 28                     | 25,776             |
| 56                     | 47,020             |
| 70                     | 48,892             |

Table 9. The number of elements of F13 pattern.

| Number of cells | Number of elements |
|-----------------|--------------------|
| 1               | 34,452             |
| 6               | 45,756             |
| 10              | 54,900             |
| 12              | 59,400             |

Table 10. The material constants of Mooney-Rivlin 5 parameters.

| Material constants | Value  |
|--------------------|--------|
| C_{10}             | -0.16808|
| C_{01}             | 0.23398 |
| C_{11}             | -2.54487|
| C_{20}             | 2.09914 |
| C_{02}             | 0.78043 |
| D                  | 0      |

4. Results and Discussion

In analyzing aspect ratio of a rectangular cross section of prism-micropillars, we found that the aspect ratio did not influence on both elastic stiffness and compressive strength of the micropillar as shown in Fig. 11-12. Figure 13 shows contour plots of deformation in z-direction. Figure 14 shows contour plots of von-Mises stress for various aspect ratios. Here, the maximum von-Mises stress occurring on the fixed surface. Figures 15-18 show the plots of compressive force and vertical displacement of F3, F4, F8 and F13 patterns respectively. We found convergence on all FE results when the number of micropillars was high enough to capture interactions between micropillars which were 84 micropillars for F3 and F4 patterns, 70 micropillars for F8 pattern and 12 cells for F13 pattern. Their contour plot of deformation in the z-direction as shown in Fig. 19. Moreover, the compressive strength of various micropillar patterns were compared and the plot of compressive pressure and vertical displacement for various micropillar patterns were shown in Fig. 20. The maximum compressive pressure were 7.73 kPa, 9.79 kPa, 5.45 kPa and 9.87 kPa for F3, F4, F8 and F13 patterns respectively. We found that F13 pattern had the highest in both elastic stiffness and the compressive strength since it had the highest loading contact area. For all micro-patterns, the collapse of micro patterns were found when the deformation was around 5 µm.

Fig. 11. Plot of compressive force and vertical displacement for various aspect ratio of prism-micropillars.

Fig. 12. Plot of von-mises stress and vertical displacement for various aspect ratios of prism-micropillars.
Fig. 13. Contour plot of deformation in the z-direction (μm) for aspect ratios of (a) 1:1, (b) 1:1.56 and (c) 1:4.

Fig. 14. Contour plot of von-mises stress (MPa) at the displacement z = -10 μm on the micropillars with (a) 1:1 aspect ratio, (b) 1:1.56 aspect ratio and (c) 1:4 aspect ratio.

Fig. 15. Plot of compressive force and vertical displacement for F3 pattern.

Fig. 16. Plot of compressive force and vertical displacement for F4 pattern.
Fig. 17. Plot of compressive force and vertical displacement for F8 pattern.

Fig. 18. Plot of compressive force and vertical displacement for F13 pattern.

Fig. 19. Contour plot of deformation in the z-direction (µm) for (a) F3 pattern, (b) F4 pattern, (c) F8 pattern and (d) F13 pattern.
5. Conclusions

For prism micropillars, the aspect ratio of the rectangular cross-section had no influence on both elastic stiffness and compressive strength. Furthermore, micropillar sheets consisting of F3, F4, F8 and F13 patterns on 150 µm thick substrate were studied on their compressive behaviors. The convergences of the FE results on the FE models of F3 pattern (84 micropillars), F4 pattern (84 micropillars), F8 pattern (70 micropillars) and F13 pattern (12 cells) on the 150 µm thick substrate were found. Here, the maximum compressive pressures of all micropillar patterns were determined as the maximum compressive pressure for which the lateral collapses of micropillars were detected. These compressive pressures were 7.73 kPa (for F3 pattern), 9.79 kPa (for F4 pattern), 5.45 kPa (for F8 pattern) and 9.87 kPa (for F13 pattern). Finally, the F13 pattern has the highest compressive strength but has the lowest WCA. To design such an effective micro-pattern, one has to optimize the loading contact area to achieve both high WCA and loading strength.

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