1	Theoretical and experimental investigation on conformal
2	polishing of microstructured surfaces
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16	Abstract: Microstructured surfaces are ubiquitous to various fields especially in
17	lighting, diffuser devices and imaging systems. While the current precision machining
18	technology can achieve conformal shapes, the finished quality of the machined surface
19	cannot be assured. Addressing this issue, this paper proposes a conformal polishing
20	method suitable to polish microstructured surfaces to achieve high surface quality while
21	preserving the shape accuracy. As part of the investigations, the damping tool and
22	profiling damping tool were developed for polishing the rectangular and cylindrical
23	surfaces. The results showed that along the direction perpendicular to the profile of the
24	micro feature, the distribution of the principal stress and velocity will change in
25	different forms at the corner depending on the shape of the micro feature. The shape
26	evolution model based on a single microfeature simulation was established by
27	considering finite slip on the workpiece surface. The simulated surface shape accuracy
28	after polishing agreed well with that obtained by the experiments. Moreover, pre-
29	machining history such as the residual tool marks and burrs were effectively removed.
30	The mean roughness (Ra) of the rectangular structure was measured as 0.4 nm and that
31	of the cylindrical structure was measured as 6.2 nm.
32	Keywords: Surface evolution, Shape accuracy, Microstructured surfaces, Conformal

33 polishing

34

35 **1. Introduction**

36 Microstructured surfaces find diverse applications in optics [1, 2]. Components such as diffuser [3], lens arrays [4, 5], and gratings [6, 7] contribute significantly to the 37 field of illumination which benefits optical components [8, 9], imaging [10, 11] and 38 39 light modulation [12, 13] to facilitate design of complex optical systems [14, 15]. As 40 the performance requirements of optical instruments continue to push the technological 41 limit, the demand for high-precision microstructured optical components is rising 42 sharply [16, 17]. Consequently, innovative manufacturing methods to achieve 43 nanoscale smoothness and submicron shape accuracy [18-20] are highly desirable.

44 Ultra-precision cutting and grinding are the two preferred methods in use currently 45 to fabricate [21-23] microstructured surfaces but are limited by the level of finishing 46 one can achieve. The complex microstructured surface with mean roughness (Ra) of 50 47 nm and shape accuracy of 0.65 µm was obtained by Wu et al. [24] through a five-axis 48 machining system. Zhou et al. [25] fabricated annular microlens arrays on Si and 6H-49 SiC substrates using an integrated microcutting-etching method by combining single 50 point diamond turning (SPDT) with ion beam etching (IBE). The surface roughness Ra 51 of microlens unit on Si obtained was 0.054 µm, and that on SiC was 0.011 µm.

Jiang et al. [26] processed microslot array, pyramid array and triangular pyramid array microstructured surfaces using an offset flying cutting servo system. The shape errors in the fabricated microstructured arrays were all below 1 μm. Guo et al. [27] fabricated V-groove microstructured surfaces using a single point diamond cutting process. The peak-to-valley (PV) shape accuracy of the V-shaped groove surface was less than 1μm and the surface roughness (Ra) was close to 15 nm.

It is known that the contact mode machining processes such as diamond machining leaves tool marks on the machined surface [28, 29], which were also observed in the investigations discussed above. While the displacement-controlled machining processes such as cutting, milling and grinding can attain high shape accuracy, they 62 cannot assure good control on the machined surface quality [30, 31]. As a result, 63 residual surface defects such as tool marks and burrs on the surface can compromise the performance of the components during their lifetime [32, 33]. For critical 64 65 components such as optical diffuser, the residual marks left by the cutting tool causes optical interference that could lead to non-uniform brightness and small-angle 66 67 scattering of light, consequently impacting the system resolution [34, 35]. For 68 microstructured surface polishing, scholars have proposed the use of pin-type wheel-69 type tools [36, 37], abrasive jet polishing [38-40], magnetic field assistance [41, 42], 70 laser polishing [43, 44] etc. However, these methods continue to pose the problems 71 related to inferior quality of the polished surface [45, 46]. Moreover, traditional 72 methods of polishing are only suitable for polishing sub-millimeter microstructured 73 surfaces [47]. Also, the rapid degradation of the polishing tool leads to rapid wear 74 during the direct contact with the workpiece. Most specifically, Jet polishing and 75 magnetic field assisted polishing have been flagged to have the problems with left over 76 of the residues of the abrasive particles [48] which causes shape errors and poor 77 performance [49, 50]. Hence, the existing polishing methods are shrouded by the 78 common problem that polishing tools are prone to wear which limits the ability to 79 maintain the surface accuracy.

80 In recent years, non-contact polishing methods based on the shear thickening 81 polishing (STP) principle have attracted a lot of attention due to the advantage of 82 process flexibility [51, 52], ease of equipment preparation [53] and cost-effectiveness 83 [54]. In recent time, Zhu et al. [51] carried out non-contact polishing using non-84 Newtonian fluid on the nickel matrix to obtain a smooth surface with a roughness (*R*a) 85 of about 3.9 nm. Li et al. [55] employed a weak chemical shear thickening polishing 86 process to polish spherical 9Cr18 parts and achieved an Ra of about 25 nm with a PV 87 shape accuracy of 1.16 µm. Wang et al. [56] polished Ti-6Al-4V biomaterial using 88 chemistry enhanced STP method. A surface roughness Sa of 7.2 nm was obtained while 89 achieving a material removal rate of 118 nm/min.

90

Zhou et al. [57] proposed a magnetic field enhanced shear thickening polishing

91 process to polish zirconia and achieved an *Ra* of about 8.3 nm. The aforementioned 92 studies demonstrate that the STP process has distinct advantages however, this method 93 in the aforementioned investigations has only been applied to planar surfaces. In this 94 regard, Li et al [58] developed an anhydrous-based shear thickening slurry to polish 95 KDP surfaces and achieved an Ra of 1.37 nm. Zhang et al. [59] developed a damping 96 tool to polish aspherical surfaces of nickel-phosphorus alloy and reported an Ra of less 97 than 1 nm.

It can once again be seen that the use of STP has been attempted only on flat [60,
61] and curved surfaces [62, 63] and its full potential to polish microstructured surfaces
is yet to be unveiled.

101 Clearly, the utilisation of non-contact method based on STP method by employing 102 non-Newtonian fluids presents significant advantages to finish optical components at 103 scale. Hence, this approach can also be extended to facilitate ultra-precision polishing 104 of microstructured surfaces. Owing to the distinctive geometric attributes of these microstructured surfaces, characterized by a substantial depth-to-width ratio, there 105 106 exists a need for sub 10 nm surface roughness while preserving shape accuracy [64, 65]. 107 Addressing this issue was the major motivation of this paper. Consequently, a 108 damping tool and a profiling damping tool for finish machining of microstructured 109 surfaces were developed as part of this investigation. A shape prediction model based 110 on a single microfeature simulation considering finite slip on the workpiece surface was 111 also developed. The result shows that the distribution of the principal stress and velocity, 112 which determine the material removal during the polishing process, changes irregularly with the change of the microstructured surface profile. The experimental results showed 113 114 that the shape error after polishing was less than 1 µm such that the surface roughness 115 of the diffuser mold converges to 6.2 nm while the roughness of the grating surface 116 decreases to 0.4 nm.

117 **2. Research methodology**

118 The material removal principle used in this study is based on the shear-thickening 119 effect of non-Newtonian fluids [66, 67], and the damping tool and profiling damping

tool were purposely designed to achieve effective polishing of microstructural 120 121 workpieces at different depth scales. The polishing tool consists of a tool base and a 122 damping pad (see Fig 1). The damping pad is affixed to the tool surface to enable 123 effective driving of the polishing slurry. Due to the presence of the damping layer, the 124 slurry can be stably driven by the designed tool, quickly reaching the peak of the 125 thickening curve and fluctuating in the highest viscosity region. Under the high-speed 126 shearing action of the tool, the slurry of the workpiece surface thickens, and the material 127 in the form of microfeatures gets removed by the particle clusters formed during the 128 process.



130 Fig. 1. Schematic of the material removal principle.

129

131 The damping and profiling damping tools were designed to polish the 132 microstructured surfaces across different scales. When damping tools were used to 133 polish structures with depths of about hundreds of micronmeters, the microfeature 134 bottom was always unable to obtain effective material removal. Damped profiling tools 135 have been developed for polishing microstructures with depths about hundreds of 136 micrometers. It should be noted that the profiling damping tool is specifically designed for array V-grooves and cylindrical structures and is not compatible with structures that 137 138 have vertical sides, such as rectangular structures. Damping tools were developed for polishing the microfeatures with depth of about a few or tens of micrometers. The 139 140 damping tool consists of a cylindrical base and a damping cloth. The function of the 141 damping cloth is to drive the polishing slurry effectively. Profiling damping tools were 142 developed for polishing the microfeature with depth of about hundreds of micrometers. 143 The profiling damping tool consists of a tool base, a soft film and a damping cloth. The

144 profiling damping tool ensures a constant gap between the tool and the microfeature



145 profile, thereby removing the workpiece surface material as evenly as possible.

146



148 3. Modelling and simulation

149 In this section, to find out the pressure and velocity field during the polishing process and the material removal distribution on the microstructured surface workpiece, 150 CFD is used to simulate the polishing process and a material removal model based on 151 152 the simulation is established. The rheological properties of the polishing slurry and the 153 finite slip condition of the workpiece surface are considered in the simulation process. 154 Based on the simulated surface pressure and velocity fields, a material removal model 155 was established to predict the surface shape of the microstructured surface during 156 polishing.

157 3.1. Finite element method

158

In the finite element modeling process, the workpiece surface was set to finite slip 159 [68]. Fig. 3 shows the velocity distribution in the gap under no slip and finite slip

- 160 conditions, and the distribution of slurry velocity u and shear force τ in the working gap.
- The workpiece surface slip velocity U_s can be expressed as 161

162
$$U_{w} = \begin{cases} 0, & \tau < \tau_{c} \\ U_{s} \left(\frac{\tau - \tau_{c}}{\tau_{n}}\right)^{m} \exp\left(-\frac{BP}{\tau_{n}}\right), & \tau > \tau_{n} \end{cases}$$
(1)

163 where τ_n and τ_c are normal and critical stresses respectively, m is a positive power, *B* is 164 a pressure coefficient and *P* is pressure [69, 70].

165 In most cases, the pressure coefficient is minimal and in processes such as 166 extrusion and lubrication flow of viscoplastic fluids and extrusion of polyethylene, the 167 contribution from this term can be ignored [71]. Therefore, the pressure coefficient B168 was set as 0 for the simulation in this paper. The exponent *m* could be 1 or larger. Based 169 on these experimental results and also to simplify the model, the positive power m was 170 set as 1.5 and the τ_n and τ_c were both set to be 5000 Pa based on the experimental results 171 when the smooth state of the workpiece surface is utilized. The value of U_s was changed 172 to simulate different magnitudes of slip.



173

Fig. 3. Schematic diagram of (a) non-slip and finite slip, (b) velocity and shear stress field in theworking gap under finite slip condition.

The finite element software ANSYS CFX was used to solve the pressure and 176 177 velocity field of microstructured surface in wedge gap during polishing [72]. Fig. 4 178 show the relationship between the tool and the workpiece as well described the 179 boundary conditions adopted for simulating the polishing process. Fig. 4(a) shows the 180 fluid domains between a single microfeature and the tool, taking the profiling damping 181 tool as an example. The tool surface was set to have no slip wall and the workpiece 182 surface was set to have a finite slip wall. The top region of the fluid domain was set as 183 open boundary, and the side region was set as symmetric boundary. The fluid domain 184 was meshed with tetrahedral elements. In addition, all relevant parameters used in the

- simulation process are shown in Table 1. the consistency coefficient was set as 0.62 Pa
- 186 s, the initial shear rate was set as 0.001 s^{-1} , the peak shear rate was set as 120 s^{-1} , the
- 187 viscosity index was set as 1.5 and the density of the fluid was set as 1450 kg/m^3 .
- 188 Table 1

Parameters	Value	
Initial shear rate γ_i	0.001 s ⁻¹	
Peak shear rate γ_p	120 s ⁻¹	
Consistency coefficient K	0.62 Pa s	
Slurry density ρ	1450 kg/m^3	
Pressure coefficient B	0	
Positive power <i>m</i>	1.5	
Normal stresses τ_n	5000 Pa	
Critical stresses τ_c	5000 Pa	
Working gap d	0.2 mm	
Tool speed <i>n</i>	600 rpm	
Tool diameter D	30 mm	

189 Parameters set in the simulation model

As shown in Fig. 4(b), the cross-sectional view of the surface meshing of single
rectangular and cylindrical microfeatures, the wedge-shaped gaps were meshed entirely.
Figure 4(c) shows the geometric dimensions of the tool and workpiece surface set
during the simulation modeling process.



195 Fig. 4. (a) boundary conditions set in the simulation and (b) grids and (c) geometry size in the

196 model.

194

- 197 *3.2. Shape prediction model*
- 198 In this section, the processing TIF and material removal distribution are modeled 199 based on the matrix data obtained from the simulation to predict the surface shape of 200 the polished microstructured surface.
- 201 3.2.1. Calculation of TIF

TIF function is an important part of deterministic polishing. Usually, the footprint of TIF is related to the pressure on the surface of the workpiece during polishing and the speed of the abrasive particle movement relative to the surface of the workpiece [73, 74]. When the pressure on the workpiece surface exceeds a certain threshold, the material yields and is removed at the same time. Similarly, the material removal in this work is related to the pressure and velocity on the nickel-phosphorus alloy material surface. But the difference is that this pressure is determined by the principal stress P_p induced by the dynamic pressure p_d and shearing stress τ . The speed is determined by the speed of the particle relative to the surface of the workpiece.

According to the von-Mises criterion [75], the equivalent principal stress P_p considering the shear stress can be estimated as

213
$$P_p(x, y) = \sqrt{p(x, y)^2 + 3\tau(x, y)^2}$$
(2)

where p(x,y) and $\tau(x,y)$ are the dynamic pressure and shear stress field in the wedge gap. The velocity field (*V*) was exported from the simulation model. Given the distribution of principal stress and velocity, the TIF matrix (*R*) can be estimated based on Preston's law[76] and R(x,y) can be expressed as

218
$$R(x, y) = K \cdot P_n(x, y) \cdot V(x, y)$$
(3)

219 3.2.2. Surface removal distribution calculation on microstructured surfaces

By determining the dwell time of the tool on the workpiece surface as shown in Fig. 5, the material removal distribution of the microfeature surface was obtained by Eq. (4) [77, 78].



223

Fig. 5. Tool path diagram.

225
$$E(x, y) = R(x, y) * *T(x, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} R(x - x', y - y') T(x', y') dx' dy'$$
(4)

where R(x,y) is the TIF of the polishing tool at the dwell point and the dwell time distribution can be written as T(x,y).

228 The discrete form of material removal distribution can be expressed as

229
$$E(x, y) = \sum_{i=0}^{I} \sum_{j=0}^{J} R(x - x'_{i}, y - y'_{j}) T(x'_{i}, y'_{j}) \Delta x' \Delta y'$$
(5)

where, *I* and *J* are the sampling points parallel to the X and Y directions of theworkpiece respectively.

The matrix solution method was used to transform the two-dimensional convolution equation into a matrix equation for solving, so formula (5) can be written in a matrix form as

235
$$[E]_{i\times j} = [R]_{i\times j} [T]_{j\times j}$$
(6)

236 Therefore, the material removal distribution matrix [E]i×1 can be expressed as

237
$$\begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_i \end{bmatrix} = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1j} \\ r_{21} & r_{22} & \cdots & r_{2j} \\ \vdots & \vdots & \ddots & \vdots \\ r_{i1} & r_{i2} & \cdots & r_{ij} \end{bmatrix} \begin{bmatrix} t_1 \\ t_2 \\ \vdots \\ t_j \end{bmatrix}$$
(7)

238 *3.3. Prediction procedure*

Fig. 6 show the flowchart of the shape accuracy prediction process. The 239 240 dimensions of the microfeature depth used for polishing were measured and the 241 damping tool or the profiling damping tool was selected based on whether its depth is 242 tens or hundreds of microns. In the CFD simulations, the tool speed n, and working gap 243 h based on the material properties of the non-Newtonian fluid slurry were used as inputs. 244 The space between the workpiece and the microfeatures was defined as the fluid domain, 245 the boundary conditions of the model were defined, and the workpiece surface was set as finite slip wall. Then, the steady state simulation of the fluid flow was carried out 246 and the calculation terminated when RMS converged to e⁻⁵. At the end of the calculation, 247 248 the post-processing was performed and the velocity and Von Mise stress value were 249 extracted to calculate the TIF of a single microfeature surface. The material removal 250 distribution was estimated based on the dwell time of the tool on the microstructured

surface of the workpiece. Finally, the profile and error of the machined workpiecesurface were estimated (see Fig 6).



253

Fig. 6. Flow chart of surface shape prediction.

255 4. Equipment and process parameters

In this section, the workpiece material object for basic experiment, the production process of polishing tools and the specific test equipment used are introduced in detail. In addition, the polishing slurry used in this experiment and the process parameters are also described in detail.

260 *4.1. Materials*

In this study, the microstructured surface in a nickel-phosphorus alloy was
obtained by ultra-precision milling process for basic experiments (see Fig 7). Fig. 7(a)
shows a rectangular micro featured workpiece with a depth of about 3 μm and a period

of 1 mm. Fig. 7(b) show a cylindrical microfeature workpiece with a depth of about
400 µm and a period of 1 mm.





Fig. 7. (a) Rectangular and (b) cylindrical microstructured workpiece prepared for the experiment. *4.2. Tool design and fabrication*

269 The damping tool and the profiling damping tool were designed to polish the 270 microstructured surfaces. In contrast to the damping tool, the profiling damping tool 271 requires a series of sequences to complete the production of the tool, before carrying 272 out the experiment. Fig. 8 depicts the schematic diagram of the fabrication process of 273 the profiling damping tool. Before conducting the polishing experiment, the initial step 274 involved aligning the polishing tool body parallel to the surface of the workpiece. In 275 the second step, the polishing tool was raised to a distance of 0.2 mm above the 276 workpiece surface in preparation for the profile replication. In the third step, the molten 277 glue was injected into the gap while rotating the tool body, and the profile of the 278 workpiece was copied. The fourth step was to trim the excess film produced by 279 replication and the prefabricated area used to bond the damping pad. In the fifth step, 280 move the profiling damping tool to the gap of 0.2 mm above the workpiece, and the 281 profiling damping tool production and position adjustment were completed.



282

283 Fig. 8. Profiling damping tool fabrication procedure.

Fig. 9(a) shows a damping polishing tool prepared for microstructured surface polishing with depth of about tens of micrometers or less. The tool surface can be seen to be covered by a damping cloth, and due to the presence of the damping cloth, the polishing slurry can be driven steadily to remove the material efficiently. Fig. 9(b) shows the profiling damping tool, whose surface is covered by equally spaced duplicated structure film and damping cloth.



- 290
- Fig. 9. The prepared (a) damping tool and (b) profiling damping tool.
- *4.3. Experimental setup and procedure*

The polishing test was carried out on the self-developed 5 degree of freedom (DOF) precision machining platform as shown in Fig. 10. The spindle installed with the polishing tools can be adjusted between 0 and 90° as required, and the rotating shaft installed with the workpiece can be adjusted to the specified angle between the workpiece and the horizontal plane according to actual needs. The relative position of 298 the workpiece and the polishing tool can be adjusted by moving the XYZ axis. The 299 slurry is transported to the polishing interface through the nozzle by the self-made blade 300 pump, and it returns to the collection pool through the tank. During the polishing 301 process, the tool axis is first set parallel to the surface of the workpiece and then the 302 tool is moved to a gap of 0.2 mm above the workpiece for the profiling procedure, and 303 finally, the tool position is adjusted by moving the profiling damping tool to 0.2 mm 304 above the workpiece. During polishing, the workpiece is fed reciprocally along the Y-305 axis, the feed speed is set to 1 mm/min, and the tool speed is set to 400-600 rpm. The 306 slurry employed in this study is a mixture of non-Newtonian fluid and silica sol. The 307 non-Newtonian fluid consists of a polyhydroxyl polymer and deionized water. The 308 abrasive size and concentration of SiO₂ are 50 nm and 10%, respectively.

309 Table 2

310 Composition of the polishing fluid and processing parameters during polishing

Composition	Content	Parameters	Value
Abrasive (SiO ₂)	10 wt%	Working gap	0.2 mm
Multi-Hydroxyl Polymer	52 wt%	Tool speed	600 rpm
Oxidant	6.5 wt%	Feed rate	100 mm/min
Deionized Water	31.5 wt%	Tilt angle	0°
		Tool diameter	30 mm



311

312 Fig. 10. (a) Schematic and (b) actual experimental set up.

313 *4.4. Measurement equipment and method*

The surface morphology of NiP alloy was observed using a super depth of field

315 microscope (VHX-600E03041132, KEYENCE, Japan) before and after polishing. The

three-dimensional topography and roughness of the workpiece surface were measured by a white light interferometer (NewView9000, Zygo, USA). The objective lens used for measurement is $10 \times (Zygo)$, the measurement and analysis range both are 400×400 µm. The roughness was evaluated using the arithmetic mean deviation (*Ra*), using a Gaussian high-pass filter with a cut-off length of 80 µm. The surface profile of the workpiece was measured using a Taylor contact profilometer (Form TalySurf PGI 840, Taylor Hobson, UK).

323 5. Results and discussion

324 The simulation and experimental results are described and discussed in detail in this section. Firstly, the velocity vector distribution of microstructured surface obtained 325 326 under the no slip and finite slip conditions are introduced. At the same time, the 327 principal stress and velocity field of rectangular and cylindrical structured surfaces 328 obtained by simulation are also introduced. Then the TIF of the proposed method and 329 the simulation results are discussed. The results of surface shape prediction after 330 polishing are compared with the experimental results, and the surface formation process 331 during polishing is illustrated. Finally, the condition before and after polishing of the 332 object workpiece and its surface roughness are shown and discussed.

333 5.1. Velocity fields comparison

334 Fig. 11 shows the velocity field and velocity vector distribution in the simulated 335 wedge gap and workpiece surface, where the workpiece surface was set as no slip wall 336 and finite slip wall respectively. Fig. 11(a) shows the velocity field in the fluid domain 337 obtained when the workpiece surface was set with a no-slip boundary condition. As 338 depicted in the Fig. 11, two vortices with decreasing speed were seen to form at both 339 ends of the wedge gap. The velocity vector within the wedge gap aligns parallel to the 340 linear velocity direction of the tool surface. It gradually diminishes from the tool surface 341 towards the workpiece, eventually reaching a velocity of 0 at any given point on the 342 workpiece surface. In Fig. 11(b), the velocity field within the fluid domain was obtained when the workpiece surface was configured with finite slip conditions. Different from 343 344 the no-slip state, the surface speed of the workpiece gradually decreases with the increase of the working gap, and the velocity direction in the gap is parallel to the tool rotation direction, and the velocity of the workpiece surface is about 0.7 m/s. The results show that using the finite slip boundary condition on the workpiece surface can reveal results close to the experimental results.



349

350 Fig. 11. Velocity field of (a) no-slip and (b) finite slip surface.

351 5.2. Principal stress and velocity fields on microstructured surface

For microstructured surfaces, surface pressure and velocity determine the material removal and uniformity, so it is crucial important to find out the distribution of principal stress and pressure on the microstructured surfaces. In this section, the principal stress and velocity distributions of flat, rectangular and cylindrical structures obtained by finite element simulation and modeling are analyzed, and the main factors affecting material removal are revealed and verified.

Flat workpiece was firstly applied in simulation and modeling programs. Figure https://www.steprincipal.stress.and.velocity.field on flat.workpiece.surface.Figure 12(a) shows the relative position diagram of the tool and the workpiece. The workpiece is flat in this part. Figure 12 (b) shows the distribution of the principal stress on the workpiece surface obtained by simulation, and Figure 12 (c) shows the cross section of the 363 principal stress distribution. As shown in the figure, on the flat surface, the principal 364 stress field demonstrate V-shaped in the Y direction, and the workpiece surface is 365 subjected to the greatest principal stress at the narrowest gap position. Figure 12 (d) 366 shows the velocity field on the flat surface, and Figure 12 (e) shows the cross section of the velocity distribution. As shown in the figure, the velocity distribution has a 367 similar trend as the principal stress, showing a V-shaped distribution, and the maximum 368 369 velocity is found at narrowest gap position. Figure 12(f) shown an interpretation 370 diagram of the principal stress and velocity distribution on the flat surface. The pressure 371 and velocity are uniformly distributed.



Fig. 12 Diagram of (a) relative position, (b)(c) principal stress, (d)(e) velocity distribution, and (f)
interpretation on flat surface.

372

375 Rectangular structure is further performed in simulation and modeling programs. Fig. 13 shows the distribution of principal stress and velocity on the rectangular 376 377 microstructured surface obtained by simulation. Figure 13 (b)(c) shows the distribution 378 of the principal stress and cross section on the rectangular workpiece surface. On the 379 rectangular microstructured surface, the principal stress field is also demonstrating V-380 shaped in the Y direction of the workpiece. However, as can be seen from the cross-381 section diagram, in the vertical direction of the microfeature (X direction), the principal 382 stress field changes at the edges and corners of the microfeature. The phenomenon of 383 increased principal stress was found at the corner of the convex, the velocity reduction

phenomenon was found at the corner of the concave part. Figure 13 (d)(e) shows the distribution of the velocity and cross section on the rectangular workpiece surface. As shown in the figure, the velocity distribution of the rectangular structure also changes at the corners of the micro features, but unlike the principal stress, the velocity shows a decreasing trend at the convex corners. Figure 13(f) is a schematic illustration of this pressure and velocity variation.



390

Fig. 13 Diagram of (a) relative position, (b)(c) principal stress, (d)(e) velocity distribution, and (f)
interpretation on rectangular surface.

393 Cylindrical structure is also performed in simulation and modeling programs. 394 Figure 14 shows the principal stress and velocity field on the cylindrical 395 microstructured surface using profiling damping tool obtained by simulation. Figure 14 (b)(c) shows the distribution of the principal stress and cross section on the cylinder 396 397 micro feature. Similar to flat and rectangular structures, the principal stress distribution 398 along the X direction is V-shaped. the principal stress field also changes at the corners 399 of the microfeature. The maximum principal stress distribution is found at the corner of 400 the end of the cylinder. Figure 14 (d)(e) shows the distribution of the velocity and cross 401 section on the cylinder micro feature. The velocity distribution along the X direction is 402 also V-shaped. The maximum velocity is also found at the end of the cylindrical 403 structure. Figure 14(f) is a schematic illustration of this pressure and velocity variation. 404 As can be seen from the figure, the maximum principal stress and velocity are both

405 concentrated at the end of the cylindrical structure. This means that more material406 removal occurs at the end of the cylinder, which is discussed in the next section.



407

Fig. 14 Diagram of (a) relative position, (b)(c) principal stress, (d)(e) velocity distribution, and (f)
interpretation on cylindrical surface.

410 5.3. Tool influence function

411 Fig. 13 shows the simulated TIF when polishing the flat, single rectangles, and 412 cylindrical surface. The TIF distribution was calculated from Eq. (6). Fig 13 reveals that 413 on the flat surface, there is a V-shaped TIF distribution, with the largest material 414 removal occurring at the narrowest wedge gap on the workpiece surface. When dealing 415 with rectangular or cylindrical microfeatures, uneven material removal can be observed 416 at the corners of these microfeatures. When the structural feature is rectangular (about 417 a few microns), most material gets removed at the sharp corners of the convex part of 418 the microfeature and relatively less material removal was observed at the sharp corners 419 of the concave part of the microfeature, and relatively less material removal occurred 420 at the sidewall area of the microfeature. For structural features that are cylindrical 421 (about hundreds of microns), the surface of the microfeatures undergoes relatively 422 consistent material removal, with slightly increased material removal occurring at the 423 corners of the microfeatures.



425 Fig. 15. TIF for single (a) flat, (b) rectangular, (c) groove structured surface.

426 *5.4. Accuracy of the profiling damping tool*

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427 To find out the accuracy of the tool during the process of polishing, the profile of the profiling damping tool was measured. Fig 14 shows the contour of the tool and the 428 429 workpiece. It can be observed from Fig 14 that the tool profile overlaps closely with 430 the profile of the workpiece. There is only a slight deviation between the depth of the 431 tool and the workpiece, and this deviation is mainly reflected in the convex part of the 432 tool. The specific deviation value was about 30 µm, which may be caused by the cooling 433 contraction of the film after replication. The working gap in the polishing process was 434 0.2 mm, and this deviation of the tool is far less than the working gap, so the impact on 435 the polishing process can be negligible.



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448



438 5.5. Shape accuracy

439 To find out the surface shape accuracy of the rectangular and cylindrical structures 440 after polishing, the profile of the microstructured surface workpiece before and after 441 polishing was measured. Fig 15 shows the calculated surface shape errors of rectangular 442 and cylindrical structures before and after polishing. The results show that the 443 theoretical and experimental results were consistent. As depicted in Fig 15(a), the error 444 before and after polishing of the rectangular structure was about 0.2 µm. The maximum 445 material removal occurred on the top corner of the rectangular structure, while lesser 446 material removal occurred on the bottom corner of the rectangular structure, which can 447 explain the reason for the edge roll-off of the rectangular structure.



Fig. 17. Theoretical and experimental errors of single (a) rectangular and (b) cylindricalmicrostructured surfaces.

451 *5.6. Surface quality*

452 To further verify the effectiveness of the proposed tool and the non-contact 453 conformal polishing method, the grating rectangular microstructured workpiece was 454 prepared for the polishing experiments. Fig 16 shows the surface observation image and 455 quality of grating rectangular before and after polishing. Fig 16(a) and (b) depict 456 microscopic images of the microstructured workpiece surface before and after the 457 polishing process. Noticeable color streaks resulting from diffraction can be observed 458 on the surface before polishing, but they disappear after the polishing process. 459 Significant differences in brightness were observed between the top and bottom 460 surfaces before polishing, and these differences disappeared after the polishing. In 461 addition, many parallel tool marks and burrs produced by cutting were observed on the 462 rectangular microfeature surface. After polishing, the surface became smoother while 463 the defects were eliminated, and the roughness decreased from the initial Ra 2.1 nm to 464 0.4 nm (see Fig 16(c)).



465

466 Fig. 18. Surface (a) observation (b) microscopic image and (c) roughness of grating rectangular467 surface before and after polishing.

468 Fig 17 shows the surface image and roughness results of the diffuser mold before 469 and after the polishing. Fig 17(a) and (b) show the images of the workpiece before and 470 after polishing. Many spiral tool marks and burrs were found on the diffuser mold 471 surface before polishing. After polishing, the surface of the mold microfeature became 472 smooth and most of the tool marks and burrs on the surface were eliminated. Fig 17(c) 473 shows the surface roughness of the mold before and after polishing. The surface 474 roughness was about 94.2 nm Ra before polishing, and the surface roughness reduced 475 to 6.2 nm Ra after polishing for 1 hour, which decreased by 93.4%.



477 Fig. 19 Surface (a) observation (b) microscopic image and (c) roughness of diffuser mold before478 and after polishing.

479 **6.** Conclusions

476

In this paper, a non-contact conformal polishing method using self-developed polishing tools to finish microstructured surfaces is proposed. The material removal and shape evolution of the workpiece surface at different scales were investigated using an integrated simulation and experimental approach. The broad conclusions can be summarized as follows:

A new damping tool to polish microstructured surfaces at depth of about a few or tens of micrometers and a profiling damping tool to polish at depth of about hundreds of micrometers were developed. These two polishing tools are demonstrated to be industrially useful for polishing array structures with complex shapes. The associated error between the profiling damping tool and the workpiece profile was below 30 μm. 490 Simulation considering the finite slip between the workpiece and the slurry was
491 configured. The pressure and velocity fields on the microfeature surface were studied.
492 Larger von Mises stress distribution and larger material removal were seen to happen
493 on the sharp corners of the top and bottom of rectangular structures and the corners of
494 cylindrical microfeatures.

495 A surface shape prediction model based on the simulation of single microfeature 496 was established. The proposed model accurately predicted the shapes of both 497 rectangular and cylindrical structures after polishing, demonstrating strong 498 corroboration with the experimental results. The shape error of the polished array 499 rectangle and cylindrical structure were about 0.3 µm and 0.8 µm, respectively.

500 The surface quality of the grating and diffuser mold taken as a testbed study was 501 improved significantly after polishing. The surface defects such as tool marks and burrs 502 on the workpiece surfaces were effectively eliminated. The surface roughness of the 503 grating has seen an 84% decrease reaching 0.4 nm, while the surface roughness of the 504 diffuser mold has decreased by 93% to 6.2 nm.

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519 Appendix A. The solving process NS equation in finite element model

520 To describe slurry flow mathematically, governing equations [79] related to the 521 conservation of mass and momentum in the fluid are applied. These equations can be 522 written in three dimensions

523 Mass conservation equation (Slurry continuity)

524
$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$
(8)

525 Momentum conservation equation

526
$$\frac{\partial p}{\partial x} = \frac{\partial}{\partial z} \left[\mu \frac{\partial u}{\partial z} \right] = \mu \frac{\partial^2 u}{\partial z^2}$$
(9)

527
$$\frac{\partial p}{\partial y} = \frac{\partial}{\partial z} \left[\mu \frac{\partial v}{\partial z} \right] = \mu \frac{\partial^2 v}{\partial z^2}$$
(10)

528
$$\frac{\partial p}{\partial z} = 0 \tag{11}$$

529 Where, u, v, w indicate the velocity in x, y, z directions respectively, p is dynamic 530 pressure, μ is the dynamic viscosity of the polishing slurry. Considering the small 531 working gaps, the thickness of the wedge gap area can be seen as a thin layer, fluid 532 behavior can be well approximated using Reynolds equation [80] combined with 533 viscosity changes. Specifically, the Reynolds equation in the working gaps, pressure p, 534 slurry thickness h and viscosity μ can be expressed as

535
$$\frac{\partial}{\partial x} \left(\frac{h^3 \cdot \partial p}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{h^3 \cdot \partial p}{\partial y} \right) = 6\mu \left[u \frac{\partial h}{\partial x} + v \frac{\partial h}{\partial y} \right]$$
(12)

536 According to the constitutive equation of non-Newtonian power-law fluids [81]

537
$$\mu = k \cdot |\dot{\gamma}|^{n-1}$$
 (13)

538 Where k is the consistency constant and n is the flow index.

539 Then the shear rate can be expressed as [76]

540
$$\tau = \mu \cdot |\gamma| = k \cdot |\gamma|^n \tag{14}$$

541 Where, γ is the velocity gradient, defined as $[82]\gamma = \nabla V = \partial V / \partial h$, $V = \sqrt{u^2 + v^2}$ is the 542 sum velocity of the xy plane. 543 Slurry thickness *h* can be defined as [83]

544

unexness *n* can be defined as [65]

$$h(x, y) = R - \sqrt{R^2 - x^2} + d$$
(15)

545 Where, R is the radius of the polishing tool and d is the polishing gap.

546 By iterative calculation with the discrete differential algorithm and Reynolds 547 equation, the stable convergent pressure can be obtained. Subsequently, the equivalent 548 principal stress P_p considering the shear stress could be calculated according to the von-549 Mises criterion.

550 Appendix B. Size parameters related to profiling damping tool fabrication

Fig. B.20 illustrates the relevant dimensional parameters for the design of the 551 552 profiling tool. The groove depth of the profiling damping tool is 0.4 mm. During the production of the replication film, there is a 0.2 mm gap between the outer circle of the 553 554 tool substrate and the upper surface of the workpiece, which means that there is a 0.6 555 mm gap between the bottom of the shaped tool groove and the upper surface of the workpiece. This precisely matches the thickness of the damping polishing pad, ensuring 556 557 that the surface of the polishing pad on the shaped tool aligns perfectly with the lowest 558 end of the replication film, without affecting the polishing process.



559

560 Fig. B.20. Dimensional information relevant to the replication film production process

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