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Graphene confers ultra-low friction on nanogear cogs

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Abstract: Friction-induced energy dissipation impedes the performance of nanomechanical devices. 31 Nevertheless, the application of graphene is known to modulate frictional dissipation by inducing 32 local strain. This work reports on the nanomechanics of graphene conformed on different textured 33 silicon surfaces that mimic the cogs of a nanoscale gear. The variation in the pitch lengths regulates 34 the strain induced in capped graphene revealed by scanning probe techniques, Raman spectroscopy 35 and molecular dynamics simulation. The atomistic visualisation elucidates asymmetric straining of 36 C-C bonds over the corrugated architecture resulting in distinct friction dissipation with respect to the 37 groove axis. For the first time, we reported experimental results for strain-dependent solid lubrication 38 39 which can be regulated by the corrugation and leads to ultra-low frictional forces. Our results are applicable for graphene covered corrugated structures with movable components such as 40 nanoelectromechanical systems, nanoscale gears, and robotics. 41

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43 Keywords: Textured surface, Graphene, Strain, Raman Spectroscopy, Frictional Force 44 Microscopy (FFM)

45 Introduction

46 Engineering nanostructure through laser texturing, ion milling and photolithography has significantly improved the sensing performance of nano and microelectromechanical systems (NEMS and 47 MEMS)^{1,2} devices by tuning wetting characteristics³, nano-channeling⁴, optical⁵, mechanical⁶ and 48 electronic properties⁷. The requirement for nano/micro-machines has surged recently, with focus 49 progressing towards miniaturized devices^{7,8}. In the field of tribology, textured surfaces with micro or 50 nanoscale dimples, grooves, pillars and other geometries are found to be beneficial for optimized 51 adhesion and friction forces⁹. Unlike macroscale textured surfaces^{10,11}, the nano-scaled structured 52 geometry pose tremendous challenges for performance and efficiency when they are in physical 53 contact with one another (e.g. gear operation at the nanoscale)⁸. Interaction forces that are relatively 54 55 weak at the macro-scale (such as van der Waals and capillary forces) become dominant at the nanoscale. Therefore, nanostructured devices are often susceptible to conditions of extreme pressure, 56 friction, and adhesion¹². The nanoscale contacts exert enormous pressure at the interface even at low 57 values of the applied normal force, subsequently leading to friction-induced wear¹³. Thus, a novel 58 59 strategy is needed to regulate these forces at the nanoscale.

Several approaches have been adapted to tune the friction force by introducing liquid-state lubricants
such as organic oils^{10,14}, ionic liquids^{15,16}, and tribological buffer layers such as polymer brushes¹⁷.
Nevertheless, the ecologically harmful effect of liquid-state lubricants¹⁸ and their inefficiency in

confined conditions related to viscosity modifications hinder their tribological performance¹⁴. A 63 potential alternative is presented by using solid-state lubricants¹⁹, in the form of nanoparticles or 64 lamellar solids such as graphite, transition metal dichalcogenide (TMD) e.g. molybdenum 65 disulfide)^{20,21} and recently reported the emerging class of MXenes (2D transition metal carbides, 66 nitrides, and carbonitrides)²². TMDs and MXenes have demonstrated impressive mechanical 67 performance and potential for possible tribological applications^{23,24,25}. One of the most promising 68 solutions to protect surfaces at the nanoscale level relies on epitaxially grown graphene and its 69 residue-free transfer technique²⁶. Graphene has the lowest bending rigidity^{27,28} coupled to high in-70 plane intrinsic strength²⁹ and is inert in humid and corrosive atmospheres³⁰. However, the substrate 71 on which graphene is deposited plays a pivotal role in modulating the mechanical, physical and 72 electronic properties of the graphene film^{31,32}. In particular, strain induced by interaction with a 73 substrate is one of the most intriguing parameters to adapt and tune graphene characteristics^{33,34}. The 74 role of substrate shape and its interfacial adhesion with graphene is theoretically studied by Wagner 75 et al. ³⁵ and observed the "snap-through" event of graphene under different textured confinements. 76 77 They presented the transformation of graphene membrane from flat to conforming states relate to its bending rigidity which is useful to regulate the strain. The induced strain or strain gradient fields^{36–38} 78 79 has a correlation with tribological characteristics of graphene and other 2D materials (MoS₂) for strain-induced lubrication²¹. In another approach, modulation of frictional characteristics in graphene 80 through functionalization (such as fluorination) is reported and hypothesized the role of flexural 81 stiffness attributed to the higher frequency of flexural phonons for enhancing frictional signals^{39,40}. 82 Nevertheless, the results are limited in the consideration of any elastic system and adhesion force 83 towards the tip apex. In the absence of functionalization, the increase in bending stiffness in 2D 84 material with adding atomic layer causes decreases in friction dissipation, as thicker graphene is lesser 85 susceptible to deform out-of-plane and ceased to adhere with tip⁴¹. Similarly, our previous work⁴² 86 demonstrated lowering of friction force for covalently bonded interface for Gr/Ni (111) than weak 87 van der Waals (vdW) Gr/Silica interface due to lesser availability of graphene towards tip apex. 88 Recently, the contact quality between suspended graphene and tip apex is altered through symmetrical 89 in-plane straining in graphene by depositing over circular-shaped textured structure in pressurized 90 conditions to achieve a super lubricating state⁴³. Nevertheless, the frictional response of asymmetric 91 strained graphene over the textured surface is a rarely addressed topic, which may play a crucial role 92 in the durability of NEMS devices. Nevertheless, the frictional response of asymmetric strained 93 graphene over the textured surface is a rarely addressed topic, which may play a crucial role in the 94 95 durability of NEMS devices.

In the present study, we investigate the interplay between texture-induced strained graphene and its 96 ability to lubricate. To do this, we employ nano-textured silicon surfaces as substrates that mimic the 97 cogs of a nanogear and use friction force microscopy (FFM) measurements in ambient conditions to 98 elucidate the effect of graphene deposition on the local friction properties. The different aspect ratios 99 (depth/pitch) of the grooves modulate the conformation/suspension of graphene, resulting in it being 100 strained. Raman spectroscopy shows the substrate-induced compressive strain in graphene over a flat 101 surface, which systematically released as pitch length decreases. Molecular dynamics simulations 102 corroborate the Raman measurements and elucidate the atomic-scale resolution of graphene 103 corrugation. Simulation results identify an asymmetric strain distribution through lattice expansion 104 and contraction of the C-C bond at different orientations. This work demonstrates, for the first time, 105 the regulation of the frictional dissipation in nanoscale architecture through strain engineering of 106 graphene. 107

108 **Results and discussion**

Atomic force microscopy (AFM) images in Figure 1(a, b, c) show the typical morphology of 109 graphene-covered textured surfaces referred to as GrP40, GrP125 and GrP250. The preparation and 110 characterisation of the textured surface is described in previous work^{44,45} and in Supplementary 111 Information S1. Each textured region comprises long parallel grooves approximately 40 nm wide; the 112 113 grooves' spacing referred to pitch length (P) varies from 40 ± 4 , 125 ± 8 and 250 ± 14 nm. A chemical vapour deposition-grown single layer of graphene has been deposited over the textured surfaces by 114 the wet transfer method⁴⁶. The topographic profiles of bare and covered surfaces, presented in **Figure** 115 1 (d, e, and f), illustrate the physical corrugation of graphene on the substrate. The measured depth 116 of the grooves is between 2.4-3nm on bare P40 and is reduced by 10-15% after graphene deposition 117 measured from bottom of trough. On the other hand, groove depths of bare P125 and P250 are ~ 4nm 118 119 and are reduced by 7-10% in GrP125 and 3-5% GrP250, respectively, revealing higher conformation depth of graphene at GrP250. For GrP40 corrugation, suspension of graphene does not reach the stage 120 of complete "snap-through"; and, a partial conformal contact is achieved³⁵. Thus, graphene can be 121 considered as a membrane clamped between two grooves that induce different strains (see 122 123 Supplementary Figure S1).



Figure1: Morphology of graphene covered textured surfaces. AFM topography of graphene covered textured surface of pitch (a) 40 ± 4 nm, (b) 125 ± 5 nm and (c) 250 ± 8 nm. (d)-(f) Topographical line profiles of bare and graphene covered textured surfaces across the grooves for covered (dark cyan) and bare surface (orange) colour. The interfacial interaction between graphene and textured surfaces of different pitch lengths through (i) conformational height, (j) strain (%) and (k) interfacial adhesion energy.

131 The conformation of graphene over the patterned surface unravel the mechanics of graphene as an act of balancing between interfacial adhesion and elastic energy stored in the graphene sheet(i.e., 132 bending and stretching)^{47,48}. The conformation induced average transverse strain (ε) and interfacial 133 adhesion energy (meVÅ-2) between graphene and textured surfaces, calculated from the height 134 profiles, are reported in Figure 1(i, j, k) (see Supplementary Information S2 for details). The 135 systematic variations in the strain values indicating the contribution from the textured surfaces for 136 their tendency to reduce compressive strain which is induced at the flat surface. The observation that 137 138 the interaction (interfacial adhesion energy) between graphene and P40 is higher derives directly from the need of compensating a larger stretching energy (due to a corresponding larger compressive 139 strain). 140

141 The substrate-induced stretching/compression of single-layer graphene and the doping for each 142 textured surface have been quantified by comparing Raman spectroscopy on the flat region (Gr/Flat)

and graphene-covered textured surfaces (GrP40 to GrP250). The Raman modes of G peak position 143 (PosG) and 2D peak position (Pos2D) are associated with strain, since a change in lattice constant 144 leads to a variation in the phonon modes. Furthermore, these modes are useful for detecting carrier 145 concentration (n) due to alteration in bond length and non-adiabatic electron-phonon coupling⁵⁰. The 146 relation between strain and doping of graphene with PosG and Pos2D is described in Supplementary 147 Information S3. It is well recognised that physically deposited graphene on a flat Si substrate results 148 in a p-type doped system under compressive strain⁵¹. The textured regions reduce the compressive 149 strain in graphene with smaller P values. This phenomenon is observed through gradual phonon 150 151 softening of G and 2D Raman modes of graphene deposited over Gr/Flat, GrP250, GrP125 and GrP40; see Figure 2a, b. Nevertheless, we did not observe the splitting of either G and 2D modes, 152 which indicates that the magnitude of the induced strain is not appreciably high $(<0.35\%)^{52}$. 153

The correlation plot in Figure 2c shows the distribution of Pos2D as a function of PosG with the 154 155 mean value of the distribution represented by stars. The strain axis and doping axis are drawn at the slope (*∂*Pos2D/*∂*PosG) range 2.25-2.8 and 0.75, respectively^{53,54}. The intersection of both axes is 156 assumed to be a point of minimal strain and doping in suspended graphene with the coordinates taken 157 from the work of Lee et al.⁵⁴. Thus, the distribution of all Raman data deviated from the intersection 158 coordinates is used to predict strain and doping values. The correlation plot illustrates a relative 159 160 change in the average compressive strain (ϵ) for Gr/flat of \approx - 0.09%, which is transformed on corrugated surfaces as follows: P= 250 nm ($\epsilon \approx -0.07\%$), P = 125 nm ($\epsilon = -0.061\%$), P = 40 nm ($\epsilon =$ 161 0.02%). This validates the argument of releasing compressive strain in graphene in the textured 162 163 regions relative to the flat surface. It is worth noting that the Raman laser spot diameter using a 100X (objective lens) is approximately 700 nm. Therefore, the measured strain and the carrier concentration 164 values are averaged over several crests, troughs, and flat regions in each spectrum. Nevertheless, the 165 distinct clusters of points in the correlation plots indicate the well-defined modulation of Raman 166 modes, and its associated strain and doping dictated by the substrate corrugation, Supplementary 167 168 Figure S2. One can get a higher spatial resolution up to 25-40 nm and enhanced Raman scattering signals through tip-enhanced Raman spectroscopy (TERS) for monitoring the contribution from the 169 individual groove of the graphene covered textured surface ⁵⁵. This technique would be useful to 170 investigate the change in the graphene lattice over the grooves and its associated electronic structure 171 172 to be considered in near future.

Unlike flat or multi-axial strained surfaces (e.g. suspended graphene over a circular trench),
corrugated surfaces can induce anisotropy in strained graphene owing to the asymmetric stretching
of carbon atoms oriented along parallel and perpendicular directions relative to the groove axis as

found by Lee and coworkers⁵⁶. The atomic-scale features of the graphene conformation over the 176 textured silicon surfaces have been investigated using molecular dynamics (MD) and density 177 functional theory (DFT) calculations of the graphene/Si at different pitch lengths, see supplementary 178 S4 for DFT and MD set-up. The crest region of GrP250 shows higher compressive strain induced 179 through contact with the Si substrate, while the neighbouring trough exhibits curvature-induced 180 tensile strain, which decreases with pitch length down to GrP40. The magnitude of the net 181 compression over a crest is proportional to the area of the graphene in direct contact with the Si 182 substrate, and is therefore higher than the tension across the trough. This leads to a decreasing average 183 value of compression, as shown in Figure 2(d), which is in excellent agreement with our Raman 184 spectroscopic measurements. A similar trend was observed by Zhang et al.⁴⁹ on biaxially strained 185 graphene covered self-assembled texturized silicon nanospheres with different diameters. In that 186 arrangement, the authors reported a transformation of compressive strain into tensile strain in 187 graphene deposited over smaller spherical particles due to the increasing real contact area at the apex. 188 Hinnefeld *et al.*⁵³ found a similar trend for graphene suspended on silicon pillars with a separation 189 190 distance of 600 nm indicating an increase in charge carrier concentration and decreased compressive strain. Here, by reducing the textured spacing by one order of magnitude (i.e. ≈ 40 nm), we find that 191 the deposited graphene potrays characteristics of both strain and doping of a partially suspended sheet. 192 193 The net height variation is illustrated in the inset Figure 2(d, see scale bar). Notably, there is a generation of ripples in the suspended region due to the release of the net compressive strain. This 194 195 phenomenon was further analyzed by FFM.



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197 Figure2: Raman spectrum of graphene covered textured region. Raman spectrum of (a) PosG (cm⁻¹) and (b) Pos2D (cm⁻¹) for graphene covered flat surface and different textured regions. (c) 198 199 Correlation plot of PosG vs Pos2D phonon modes for deconvoluted strain and doping in graphene from flat to the textured regions. The data distribution is from 50-70 Raman spectra and the mean 200 201 values are represented by star-shaped points. The strain (ε) and doping (n) axis classify the 202 distribution of Raman data. (d) The bond strain distribution at the crest, trough and averaged over the entire surface (black colour data) for different pitch lengths measured from MD simulations. Inset 203 shows the net height (Z-scale) variation at crest and trough regions for GrP40 under the influence of 204 net tensile and compressive strain. 205

As Raman analysis suggests that the Gr/Flat and GrP(40) configurations provide the most pronounced differences in strain values, these extreme surfaces were chosen for FFM⁵⁷ measurements. Due to the intrinsic anisotropy in the texture-induced strain in graphene, FFM measurements were performed in orthogonal (**Figure 3a-c**) and parallel (**Figure 3d-f**) directions relative to the groove axis of GrP(40)

(details about procedure and calibration are reported in Supplementary Information S5). The FFM 211 images on the GrP40 sample comprises bare textured silicon regions and nearby graphene covered 212 areas in a single acquisition. In this way, bare and covered textured surfaces are compared under 213 214 similar contact conditions, so that the local environment and possible geometrical effects or tip shape contributions can be disentangled (see Figure S5 for estimation of tip curvature radius). There is a 215 significant contrast in the lateral force values between bare and covered graphene for both orientations 216 (Figure 3b, e), which evidences the excellent lubrication performance of single-layer graphene over 217 the periodic surface. The presence of graphene reduces the average friction force up to 10 times 218 219 compared to the bare surface under similar applied load conditions ranging from 10-30 nN, with no edge failure noticeable. These results are in agreement with previous nanotribological 220 characterizations of graphene on flat silicon substrates^{58–60} and lower than crystal and polycrystalline 221 CVD MoS_2^{25} and comparable to hBN/silica⁶¹. The lateral force profile in **Figure 3c** shows a markedly 222 distinguishable undulated friction force response between graphene-covered and bare silicon, 223 224 orthogonal to the groove axis. Here, the lateral force is significant with stochastic variation over the 225 bare silicon but is reduced and periodically modulated in the graphene capped region.

226 While scanning parallel to the groove axis at the capped region, friction force modulation as a function of tip displacement is almost zero, though stochastic lateral force is sustained at the bare surface. This 227 is clearly illustrated in the lateral force map in Figure 3e and in the profile drawn orthogonal to the 228 groove axis (Figure 3f) to provide a valid comparison with Figure 3c. The detailed analysis between 229 crest and trough for the scanned orthogonal and parallel reveals a remarkable difference (Gr/LF_{Trough} 230 parallel -Gr/LF_{crest parallel}) ≈ 0.2 nN and (Gr/LF_{Trough orthogonal} -Gr/LF_{crest orthogonal}) ≈ 1.5 nN; a more than 231 seven-fold increase. The ratio of the friction force at trough/crest measured during the scan in parallel 232 233 and orthogonal directions at fixed load conditions is ≈ 2 and 5, respectively. Thus, the trough region 234 of an orthogonally-scanned textured surface contributes to the highest lateral force, but this effect is 235 suppressed along the parallel-scanned region. On the other hand, the frictional response over the bare 236 Si textured surface scanned in orthogonal and parallel directions is isotropic, as expected for this design of texturing⁶². This indicates that the anisotropic strain distribution in the graphene monolayer 237 plays a pivotal role in regulating the friction force induced from the textured surface. 238

The texture induced straining in graphene, undulating friction dissipation and anisotropic sliding resistance over the groove axis could be useful in regulating the motion of nanoscale objects, in engineering designer diffusion gradients for adsorbed molecules or even as a smart substrate to effect the proliferation of biological cells for tissue engineering applications. Such a high degree of friction force regulation is not possible over flat surfaces coated in graphene, which shows similar friction force (isotropic) in different scanning directions, see Supplementary Information (Figure S6). While,
 frictional anisotropy is also reported through different arrangements of carbon atoms in graphene^{63,64},
 here we demonstrate friction force regulation through the graphene-covered textured substrate as a
 versatile post-treatment for surfaces in nanomechanical devices.





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Figure 3. Effect of scan direction on friction force for GrP(40). First row shows (a) topography 250 image (1.0 x 1.0 micron) and (b) lateral force map (1.0 x 0.3 micron) measured at applied normal 251 load ≈30nN on GrP40 for grooves axis aligned orthogonal to the fast scan direction. The white dashed 252 line in topography profiles represents the interface between the bare and graphene covered region. (c) 253 Top, height profile (orange colour corresponds to bare silicon, dark cyan colour to graphene covered 254 region) and, bottom, corresponding lateral force profile extracted from black dashed line in (b). 255 Second-row shows (d) topography image (1.0 x 1.0 micron) and (e) lateral force map (1.0 x 0.3 256 micron) measured on GrP40 for groove axis aligned parallel to the fast scan direction at applied 257 258 normal load ≈ 25 nN. (f) Top, height profile and bottom, corresponding lateral force profile extracted from black dashed line in (e). 259

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The load dependence friction curves for P(40) and GrP(40) are reported in **Figure 4** for orthogonaland parallel-scanned directions (see details in Supplementary Information **S6**, **Figure S7-S9**). The friction force values for the bare textured region are increased by a factor of 10 as compared to graphene-covered regions for all applied loads range (-10 to 30 nN), consistent with the lateral force

profile. The shear strength (S = friction force/area) of the interface is measured by fitting the data 265 through the Derjaguin-Muller-Toporov (DMT) model (continuous line in Figure 4 (a, b)) following 266 2/3 power law within continuum mechanical modelling of the contact region^{65–67} and the coefficient 267 of friction (COF) is measured by a linear fit of the curves (dashed lines). The use of DMT 268 approximation is justified due to low adhesion force at the interfacial contact. Nevertheless, these 269 contact conditions could alter depending on the magnitude of local adhesion force, where different 270 contact conditions (e.g. Johnson-Kendall-Roberts (JKR)) can be implemented as reported by Deng et 271 al.⁵⁹ and Lang and coworkers⁶⁸. The results are shown in **Figure 5**, revealing a factor of three change 272 in the S(MPa) for GrP40 between parallel and orthogonal directions to the groove axis ($38/12 \approx 3.16$). 273 In contrast, S measured for bare P40 for scanned parallel and orthogonal directions found comparable 274 $(345/322 \approx 1.07)$. Also, S measured for sliding parallel to the groove on GrP40 (S ≈ 12 MPa) is lower 275 by $\approx 50\%$ than Gr/Flat (for S ≈ 25 MPa), which is in good agreement with the literature ^{59,69}. 276

The COF values are corroborated with S revealing minimal values of 0.009±0.001 and 0.011±0.002 277 at different locations respectively. The COF values for the Gr/Flat surface was found to be 278 intermediate between the orthogonal and parallel scanned axis. Our results are in good agreement 279 with the investigation presented by Zhang and coworkers⁴³ on tuning the COF by regulating strain in 280 the suspended graphene. The reported COF of the suspended graphene (a region of low strain) is 281 almost double compared to that of strained (0.3%) graphene. The presented textured surfaces 282 demonstrate that crests and troughs serve as distinct strained regions that can regulate the friction 283 force. The FFM values for Gr/Flat represent a compressive strain system, as demonstrated in the 284 Raman correlation plot. Here, sliding of tip under finite normal force leads to elastic buckle formation 285 as a "puckering" effect which leads to the higher friction force values⁴¹. 286

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Figure 4: Friction Force as a function of load applied to groove axis and strain distribution: 290 Experimental data of load dependent friction force curves on GrP40 sample with the grooves axis 291 292 oriented parallel (blue) and perpendicular (red) to the fast scan direction; (a) on bare silicon textured surface (b) on adjacent graphene covered region. Square and circular shaped data represent the 293 294 experimental values, continuous lines are the fitting curve from DMT model and dashed line is the linear fit. (c) MD simulation of a graphene sheet sags into the P40 textured Si surface. The vertical 295 296 drawn dashed green lines represent the trough region of suspended graphene between two crests. (d) Strain distribution based on bond strain variation along the x-axis (Δx), (e) y-axis (Δy) and (f) total 297 298 bond length (b_0) . The Inset region (marked by the coloured rectangle in panel (f)) shows the variation in C-C bond length in the crest and trough regions. The asymmetry in b₀ between different regions 299 and along different axes is readily apparent, as shown in the zoom-in image. 300

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The anisotropic values of the friction force for the graphene covered textured surface can be explained through anisotropic stretching/compression of C-C bonds in orthogonal directions over an individual groove. It has been validated through MD simulation for graphene over P40 architecture, as shown

in Figure 4 (c). The carbon-silicon interaction has been implemented using a Lennard Jones 6-12 305 potential with ε (Si-C) = 8.909 meV and σ (Si-C) = 0.3326 nm to model physisorption of the graphene 306 monolayer on a silicon substrate $\frac{70,71}{1}$. The strain distribution in graphene over the crest and trough 307 (between green dashed lines in panel (c)) in orthogonal (x), parallel (y) and out-of-plane to the silicon 308 surface has been calculated through percentage changes in Δx , Δy and bond length b_0 = 309 $\sqrt{\Delta x^2 + \Delta y^2 + \Delta z^2}$ with respect to Gr/Flat (see Supplementary Information S4 for details) 310 respectively, and is shown in Figure 4 (d, e, f). Along the x-axis, the carbon atoms of graphene at a 311 crest are continually stretched until the crest-trough interface is reached (red colour). The localised 312 313 stretching of C-C bonds at the interface leads to a net compressive strain distribution at the trough of equal magnitude, see scale bar at Figure 4 (d). Along the y-axis, the crest region weakly compresses 314 the C-C bond in contrast to the Δx strain distribution, but a significant tensile strain dominates from 315 316 interface to the trough region. Thus, there is a net tensile strain resulting from the combined effect of substrate adhesion and adjacent suspended graphene, see Figure 4 (e). 317

The integral bond length (b_0) distribution at the crest illustrates asymmetric bond alteration along the 318 orthogonal (stretching) and parallel (compressive) directions relative to the groove axis. This 319 asymmetry is also sustained at the trough, but a higher magnitude observed (see Figure 4(f)) and its 320 inset marked by rectangles). Thus, the friction force is lowest whilst sliding perpendicular to the 321 stretched axis of graphene. Also, this distinction in the bond length distribution results in anisotropy 322 323 in friction forces orthogonal and parallel to the groove axis. It clearly shows the remarkable anisotropic tribological (friction force, COF, S) performance of graphene over the same textured 324 325 surface, which is not possible for a traditional Gr/Flat system. Thus, graphene covered textured systems could bring an era of tuned friction force in nanoscale, which has been a non-trivial task in 326 327 the last decades. Moreover, such regulated friction could enhance the performance of nanomachines.

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Figure 5: Shear strength (MPa) and COF values of nanogear. The modulation in the shear strength (S, MPa) and COF values at different scanning directions. Graphene on a flat surface lies intermediate values between scanning parallel (||) and perpendicular (\perp) to the groove axis.

333 Conclusion

In summary, the deposition of graphene over textured silicon surfaces can offer a wide range of 334 opportunities due to the interplay between adhesion force energy, bending, stretching, and strained 335 orientation. By controlling the groove separation distance in the substrate, a tuneable strain in a single 336 layer of graphene can be achieved, presented through the analytical modelling, MD simulation and 337 Raman spectroscopic measurements. The graphene deposited over a flat Si surface undergoes 338 compressive strain, which is released over the textured surfaces. The overlayered graphene also drops 339 the friction force values at the extent of extreme lubricity and channelizes the friction dissipation 340 while sliding, complementary to the textured geometry. The strain distribution in graphene over the 341 342 textured architecture regulates the friction force; consequently, COF and S values. Thus, single-layer 343 graphene deposited onto an anisotropic nanotextured system could acquire diverse nanomechanical 344 properties. It is demonstrated in reference to the FFM that depends on the sliding direction with respect to grooves orientation. The presented work will pave the pathway to nanoscale devices for 345 346 efficient functioning and controlled motion of nanoscale objects, particularly in nanomechanical devices and nanorobotics. 347

348 Materials and Methods Section

Deposition of graphene over textured surface: Commercially available single-layer CVD graphene 349 from ACS Material (Pasadena, CA-USA) and Graphenea Inc. (Spain) were deposited on 350 nanostructured surfaces through the standard method of polymer assisted wet transfer followed by 351 removal of polymer residue in an acetone bath (40°C for 30 min). Later, samples were dried in the 352 oven at 40°C for 20 min and sequentially heated in a vacuum at 300°C for 2 hrs. The validation of 353 distribution of single graphene layer is carried out by Raman spectroscopy through an intensity ratio 354 355 of 2D/G > 1.3. AFM assisted mechanical cleaning have been conducted by a sacrificial cantilever prior to the friction measurements. 356

Raman measurements: Raman Spectroscopy is carried out by using a Renishaw inVia confocal Raman microscope. The laser line used for the investigation was $\lambda = 532$ nm (Source: Solid-state, model RL53250) and 1800 groove mm⁻¹ grating. All the measurements were performed at 10% laser power (controlled through ND filters) with 5 second exposure at 100X magnification. This set-up can provide the spectral resolution up to 0.3 cm⁻¹ and the penetration depth up to 0.7-0.93 µm for Si wafer⁷², which is sufficient for our investigation. The Raman modes of G and 2D peaks are fitted with Lorentzian curve to evaluate the peak positions (cm⁻¹) and peak intensity.

Atomic force microscopy and Friction Force Microscopy: Two different Atomic Force Microscope (AFM) were utilized during the experiments. The Bruker Dimension Icon with Peak Force Tapping ModeTM option and the NT-MDT NTEGRA AURA system. All the measurements were carried out in air, under ambient conditions. Commercially available rectangular shaped silicon cantilevers

368 (MikroMaschHQ: CSC37/NoAl) with nominal normal elastic constants between 0.2 and 0.8 N m^{-1}

- 369 were used for Friction Force Microscopy (FFM) measurements. The detailed calibration procedure
- 370 for the measurements is mentioned in supplementary S5.

371 Acknowledgement:

M.T. and A.B.D. would like to acknowledge strategic development funding from the University of 372 Sussex. J.G.M. acknowledges the use of the HPCMidlands+ facility, funded by EPSRC grant 373 EP/P020232/1 as part of the HPC Midlands+ consortium. P.M.A. acknowledges support from the Air 374 Force Office of Scientific Research under award number FA9550-18-1-0072. A.M. and G.P. like to 375 acknowledge support from MIUR, PRIN 2017 project n.2017PZCB5 - UTFROM; A.R. G.P. and 376 S.V. like to acknowledge support from Regione Emilia Romagna, Project INTERMECH and Project 377 n. PG/2018//631311-RIMMEL. N.M.P. has received funding from the European Union's Horizon 378 2020 Research and Innovation Programme under grant agreement GrapheneCore3 n. 881603.We 379 thank G. Gazzadi (CNR-Istituto Nanoscienze) for P125 and P250 substrate sculpting by Focused Ion 380 381 Beam.

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