Solvent-free optical recording of structural colours on pre-imprinted photocrosslinkable nanostructures (supporting information)

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1. Micrographs of nanostructure arrays
Figure S1: Micrographs of nanostructure arrays. (a) Schematic layout of pixel bands and the SEM image of the pixel bands on the quartz stamp. (b) – (d) AFM images of nanowell arrays on R, G and B band of the quartz stamp, respectively. (e) – (g) AFM images of SU-8 nanocone arrays thermally imprinted from R, G and B band, respectively. (h) – (j) AFM images of SU-8 nanocone arrays after UV exposure and 2-step heating, from R, G and B band, respectively.
2. Photomask pattern generation for patterning full-colour images

The photomask pattern for contact photomask exposure was generated using a custom-written MATLAB script. The process is illustrated in figure S2. The target colour image was loaded into the program and the program automatically adjusted the image size, resolution and orientation according to the layout of pixel bands. The R, G and B pixel bands are periodically arranged into 1-D array with 25 μm center-to-center distance. Each effective pixel is considered as a square in size of 75 μm × 75 μm. The size of each subpixel is thus 25 μm × 75 μm in size. The colour to be displayed on each effective pixel is determined by the area of the produced rectangular apertures on R, G and B subpixel. For example, to pattern the purple lines in the image ([R, G, B] = [112, 48, 160]), the generated rectangles on R, G and B subpixel are 13.3 μm × 49.7 μm, 8.7 μm × 32.5 μm, and 15.8 μm × 59.4 μm, respectively. It should be noted that there exist about 2 μm ~ 4 μm wide gaps between two adjacent bands, which is an artifact of the LIL process in fabricating the quartz stamp. Considering the gaps, a full white pixel ([R, G, B] = [255, 255, 255]) is translated into three 20 μm × 75 μm rectangles on corresponding subpixels to display the maximum subpixel brightness. Therefore, the produced rectangles for aforementioned purple colour can effectively be read out as [R, G, B] = [44%, 19%, 62%] of maximum subpixel brightness from the patterned pixels on the pixelated nanocone arrays.

Figure S2: Process to generate a photomask pattern according to an input colour image.
3. Numerical modelling of flow of polymer above glass transition temperature

Comsol multiphysics 5.2a, which is a finite element method (FEM) based software, was employed as the modelling code in this study. The surface dynamics of the nanoimprinted polymer fluid reflow during the course of melting was investigated using the microfluidics and moving mesh interfaces. Remeshing of the evolving boundaries of the flowing resist elements through Arbitrary Lagrangian Eulerian (ALE) interface allows for temporal and spatial analysis of the process. The actual 3D) nanopillar structure was numerically analyzed in 2D axisymmetric regime for simplification purposes providing significantly reduced run time and required memory and thus lowering the computational costs.

In this preliminary simulation, polystyrene (PS) is studied instead of SU-8 due to the known material parameters of the former. The property of partially crosslinked SU-8 is not sufficiently known yet. In our future work, we will apply simulations on SU-8. The 2D axially symmetric conical PS nanopillar structure has a 240 nm base radius and a 280 nm height, laid on a 1 um-thick residual layer. PS with a density of 2330 Kg/m³ and Tg~103 °C [1] was considered as the melting thermoplastic polymer for implementing the rheological dynamics studies at ~118 °C (Tg+15°C) with a dynamic viscosity of 551×10⁴ Pa.s [1]. Thermal conductivity of PS was obtained from [2]. The two-phase fluid flow provides the possibility of studying the surface tension along with the opposing damped viscous forces on the Newtonian polymer fluid flown in air through linearized Navier-Stokes equation, where we neglect the nonlinear inertial terms to examine the creeping flow of the incompressible fluid with low Reynolds number. Using the so-called Stokes equations with properly defined boundary conditions and decently meshed structure, the pressure and velocity fields were computationally derived and the temporal surface profile of the levelling process was obtained consequently.

Free deformation was activated on the entire geometry domain. The lateral and bottom boundaries of the residual layer were postulated to have zero mesh displacement in the r and z directions, respectively, while a surface tension equal to 34 N/m [1] was applied on the top surface boundaries. Further, a symmetry boundary condition was used on the bottom boundary and no-slip boundary condition was applied to the right wall, between the polymer and the air. The effect of gravity on the pattern flow was ignored due to the small dimensions and large surface to volume ratio of the nanostructures. By applying finer sized triangular meshes, fairly good and convergent results were achieved considering the trade-off between the mesh size and the required simulation time and memory.
Figure S3: Simulation of thermoplastic flow of a polystyrene nanopillar. (a) Simulation configuration with geometry and boundary conditions. (b) Mesh used in simulation. (c)-(f) Simulated thermoplastic flow of PS after 0 ms, 33 ms, 66 ms and 100 ms, respectively.

References:
