Electronic Supplementary Material (ESI) for Lab on a Chip.

Supporting Information

Solvent Immersion Imprint Lithography

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Further Information on the Molecular Dynamics Simulation

The molecular dynamics simulations were performed on a system consisting of 200 polystyrene and 1000 acetone or chloroform in a rectangular simulation box with lateral dimensions of 51.6 x 51.6 Å. The initial configuration of the system was obtained by joining two bulk liquid slabs, which have been equilibrated separately to give the correct bulk liquid densities. We first minimized the total energy of this initial structure to remove the excess initial strain. After energy minimization, we follow the system evolution for 100 ns at a constant volume and temperature (NVT ensemble). During the entire simulation, periodic boundary conditions were applied in all three spatial directions. A molecular cutoff distance of 10 Å was used for Lennard-Jones interactions. The particle mesh Ewald method was employed to handle the long-range Coulombic interactions [30]. The temperature of the systems was maintained at 300 K using the Langevin dynamics thermostat [31]. The SHAKE algorithm was used to constrain all the bonds involving hydrogen atoms and a time step of 2 fs was used to integrate the equations of motion.

Figure S1

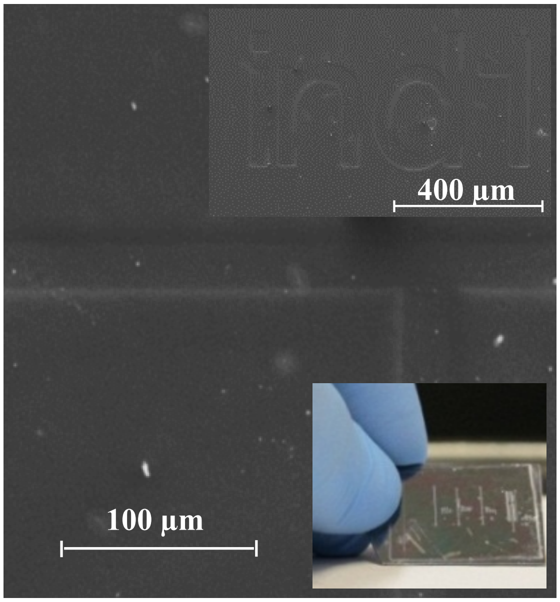

Figure S1: An SEM image of an imprinted polystyrene film spun on a silicon substrate; the imprinted feature depicts a junction of two microchannels, while the imprinted depth was approximately 5 µm. The inset shows a larger scale feature of certain imprinted characters on the same film.

Figure S2

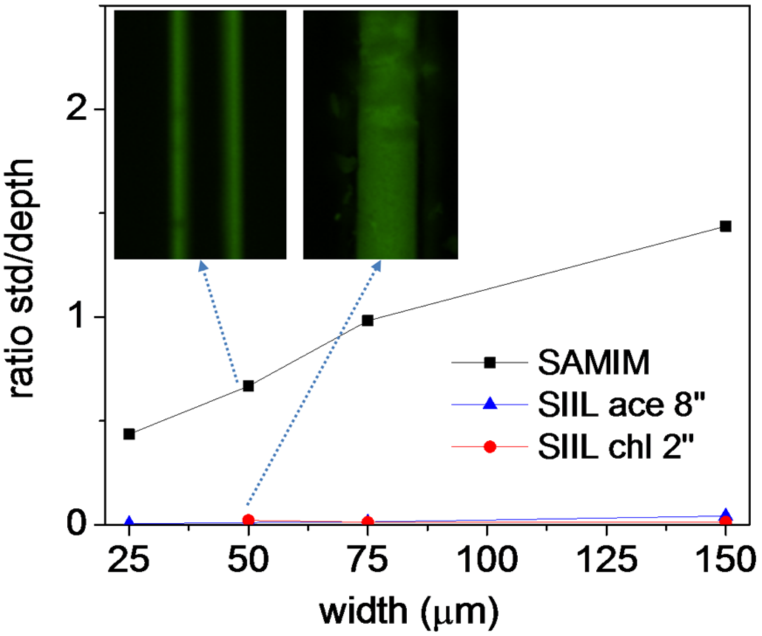

Figure S2: The ratio of the standard deviation of the imprinted depth over its mean value as a function of the imprinted feature width for SAMIM and directed polymer dissolution in acetone and chloroform; inset shows the depth profile for SAMIM and dissolution in acetone, as well as fluorescent images of thermally imprinted and thermally bonded channels fabricated with each method. The molded morphology in SAMIM suggests that the solvent is trapped at the edges of the stamp's protrusion, leading thus to primarily to edge effects. This effect was more pronounced for deeper and wider features, and was not observed in the case of SIIL.

Figure S3

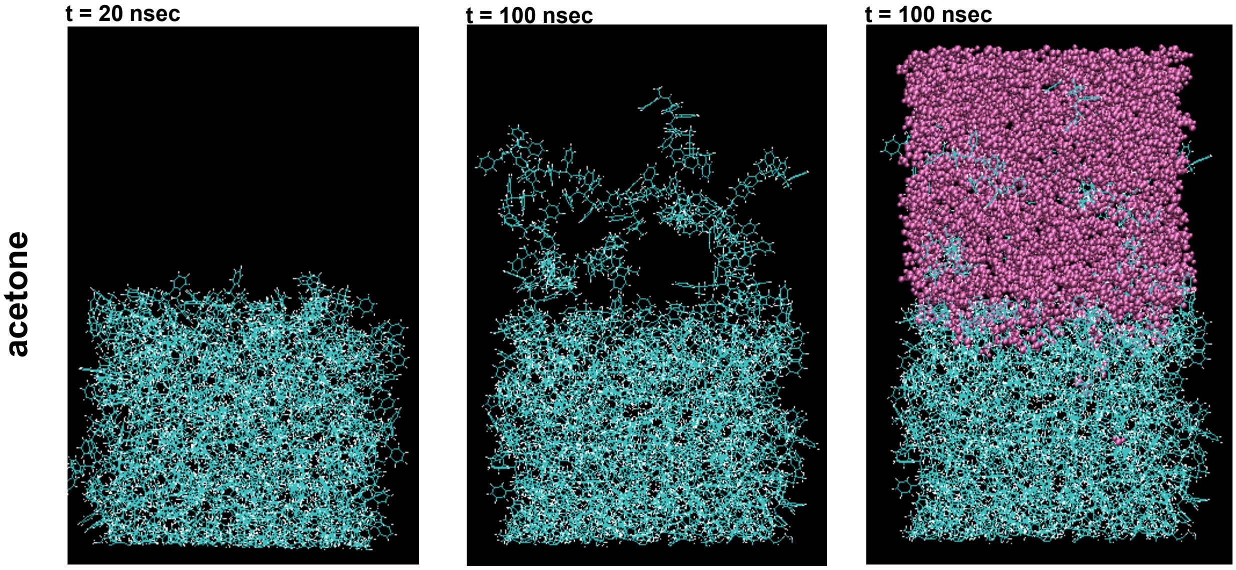

Figure S3: Molecular dynamics simulations of the polystyrene - acetone interactions. The polymer is shown in blue, and the solvent in purple. Two timeframes were chosen, one at 20ns and another at 100ns, showing the dissolution of the polymer chains, and the penetration of the solvent into the polymer matrix.

Figure S4

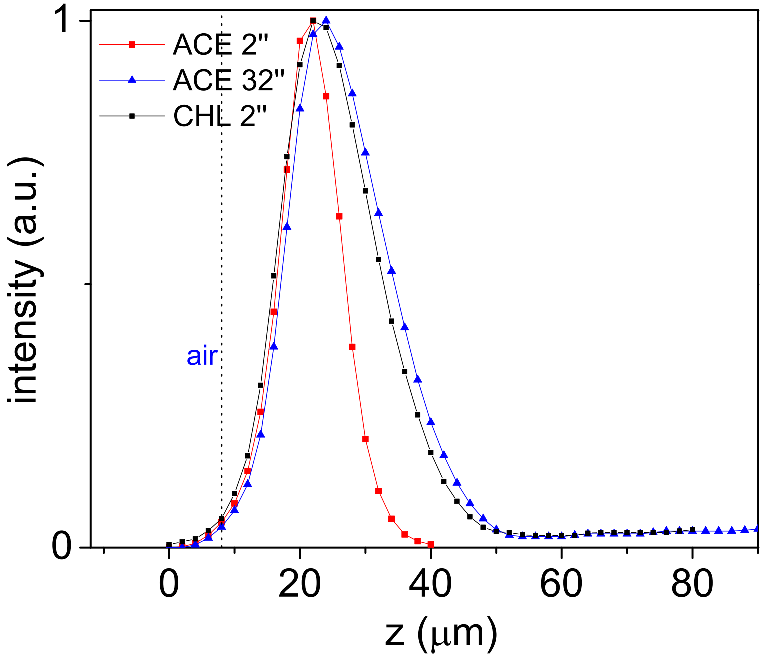

Figure S4: Confocal intensity measurements across the depth of the surface gel formed through PS immersion in stained acetone and chloroform for different durations. The gel layer fluoresces within a finite layer, with a characteristic Gaussian shape due to the finite confocal resolution. Additionally, the fluorescence does not return to zero at high depths, especially for longer solvent exposures (Figure S7). This suggests that under these immersion conditions, the solvent penetrates past the gel, filling the voids in-between the polymer chains without creating new ones.

Figure S5

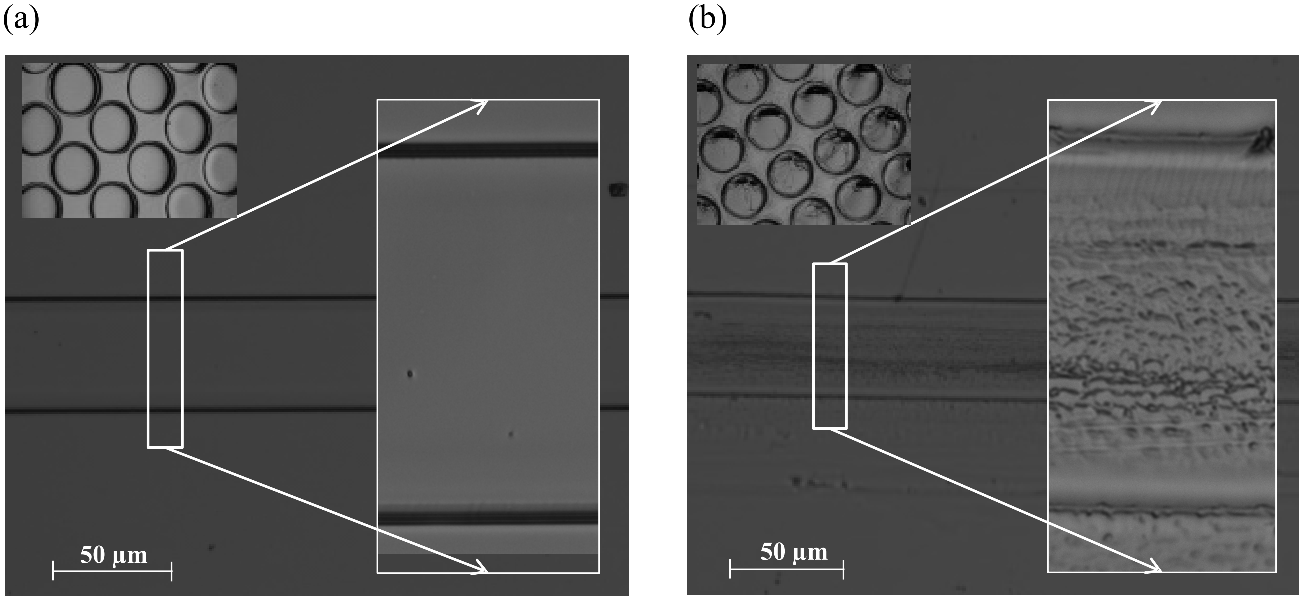

Figure S5: Bright field microscopy images of imprinted PS surfaces subsequent to their interaction with different vapor pressure solvents, namely acetone (a) and gamma-Butyrolactone (b).

Figure S6

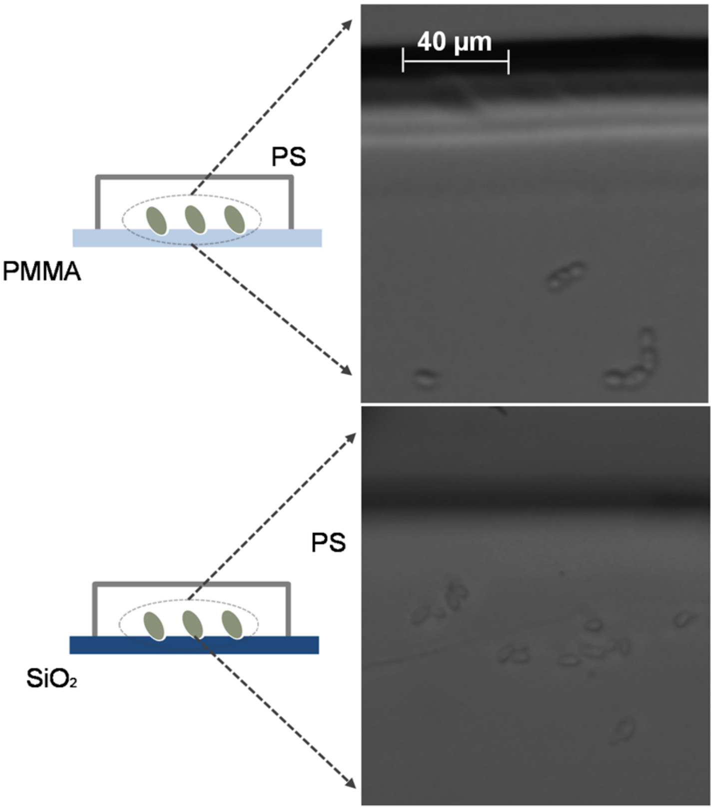

Figure S6: Heterogeneous polymer microfluidics; the upper half depicts a PS microchannel bonded with a flat PMMA film; the microscopy image depicts Yarrowia Lipolytica cells adhered on the PMMA surface. The lower half illustrates the same as the upper, however the bottom surface is silica.

Video S1: A video illustrating the imprinting and assembly process of a micro-scale pore model in polystyrene by an 8 sec immersion in acetone. Subsequent to bonding, an ethanol solution of fluorescein is employed to fill the micromodel and to better visualize the microsystem under a UV lamp. The video is displayed in real time, maintaining only frames that illustrate the process.

Video S2: A FLIM video illustrating the effect of gaseous oxygen diffusion on the lifetime of a phosphorescent sensor implanted in a SIL imprinted, and sealed optofluidic chip. In the video, the intensity of each pixel denotes phosphorescence lifetime (bright is equal to high lifetime). The video rate is one frame per 30 sec.