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

Supporting information

A portable microfluidic device for thermally controlled granular sample manipulation

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Electronic Supporting Information (ESI)

Section S1. The geometrical structure of the portable microfluidic device for particle and droplet manipulation.

Section S2. Fabrication process of ITO-made microheaters

Section S3. Schematic of the microchip for droplet generation.

Section S4. Theoretical background for thermally controlled particle and droplet manipulation.

Section S5. Numerical model and its boundary conditions

Additional Supplementary Material (AVI):

Video S1: Operation of the microfluidic device and silica particle focusing

Video S2: Silica particle focusing

Video S3: Yeast cell focusing

Video S4: Single particle migration under the energization of a single strip microheater

Video S5: Single particle migration under the energization of two adjacent strip microheaters

Video S6: Single-core double-emulsion droplet release

Video S7: Dual-core double-emulsion droplet release.

Section S1: Geometrical structure of the portable microfluidic device for particle and droplet manipulation

1. Microfluidic device.

The geometrical structure of the microfluidic device for particle and droplet manipulation is shown in **Figure S1.**

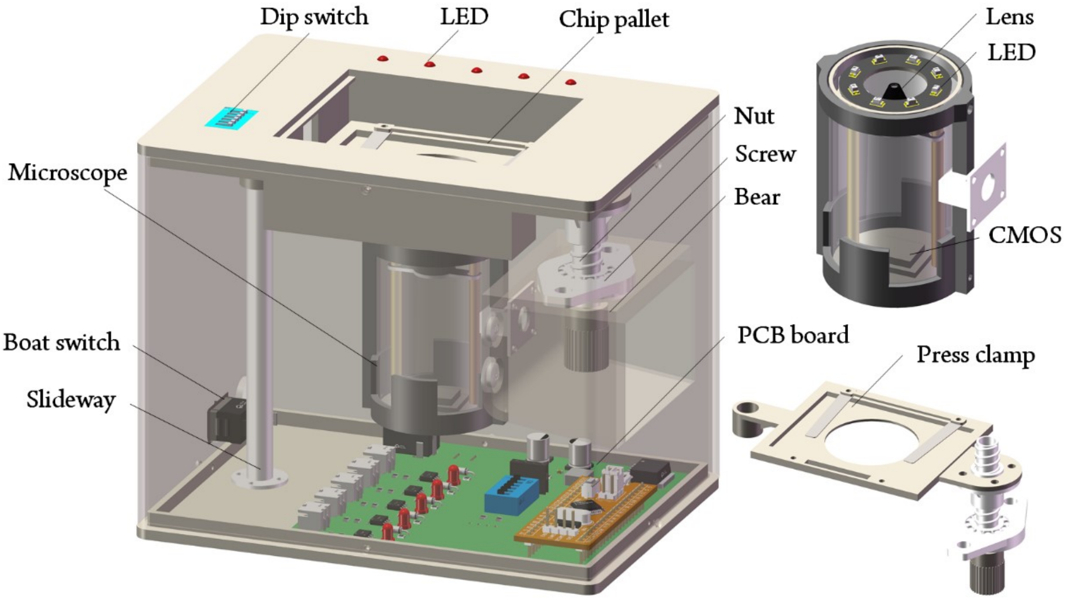

Figure S1. The microfluidic device for particle and droplet manipulation

2. Microfluidic chip

The geometrical structure of the microfluidic chip for particle and droplet manipulation is shown in **Figure S2.**

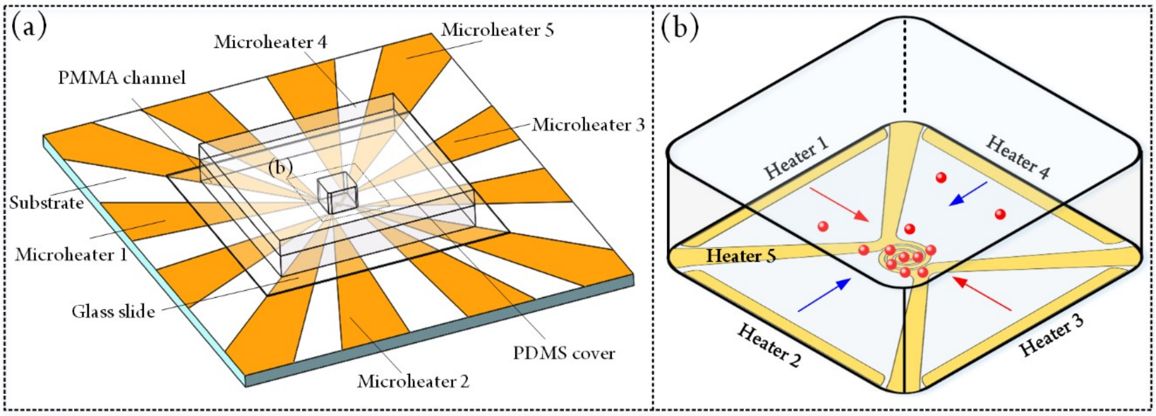

Figure S2. The geometrical structure of the microfluidic chip for particle and droplet manipulation

Section S2: Fabrication process of ITO-made microheaters

The microheaters in this study are fabricated by enriching commercial glasses with 1.2-μm thick ITO films. The schematic of the fabrication steps is shown in Figure S3.

1) a glass substrate with an ITO film (South China Xiangcheng Technology Co., LTD, China) is cleaned first and dried at 120 °C for 15min, then the positive photoresist AZ4620 is coated on an ITO substrate at 500 rpm for 15s followed by 4000 rpm for 45 s (Figure S3 a).
2) A soft bake process of ITO glass with AZ420 film is performed at 100 °C for 6 min, then the photoresist was exposed to the UV light of an exposure machine for 180 s (Boda Technology Co. LTD, Chia) (Figure S3 b). The state of the photoresist film is shown in Figure S3 c).
3) The ITO substrate is developed in an AZdeveloper solution (NMD-W, 2.38%) for 30 s, the photoresist with exposure will be removed (Figure S3 d).
4) The electrode structure is obtained by etching the ITO glass with HCl solution (~20% HCl and ~2 wt % FeCl3) for 6 min (Figure S3 e).
5) Finally, the microheater can be obtained after removing the residual photoresist using acetone (Figure S3 f).

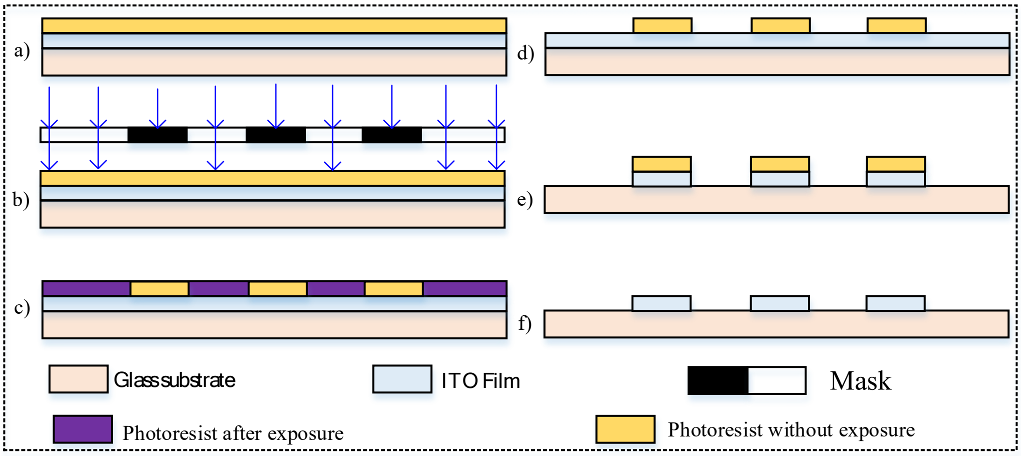

Figure S3. Schematic of the fabrication steps of the ITO-made microheaters

Section S3: Schematic of the microchip for droplet generation

1. Chip for HDDA droplet template generation

The geometrical structure of the microchip for HDDA droplet template generation is shown in **Figure S4**

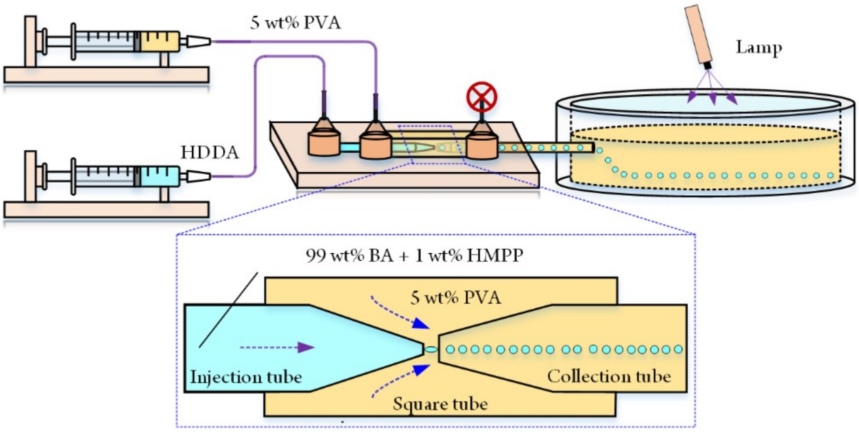

Figure S4. Schematic of the chip for HDDA droplet generation

2. Chip for double emulsion droplet generation

The geometrical structure of the microchip for double-emulsion droplet generation is shown in **Figure S5**.

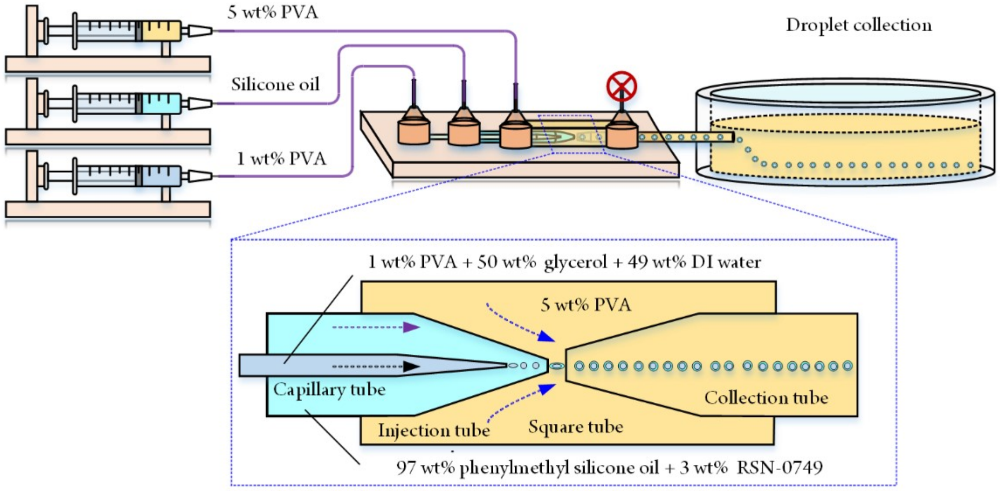

Figure S5. Schematic of the chip for double-emulsion droplet generation

Section S4: Theoretical background for thermally controlled particle and droplet manipulation

The basic theories for thermally controlled particle and droplet manipulaiton include three parts: heat transfer in microchip, fluid convection and particle migration.

1. Heat transfer.

ITO-made microheaters are the heating sources of the microsystem, and their temperature distributions meet the following equation,

$$\rho_I c_I \frac{\partial T}{\partial t} = \nabla \cdot (k_I \nabla T) + q \tag{S1}$$

where, ρ_I is the density of ITO film, c_I the heat capacity, k_I the thermal conductivity, q the Joule heating source.

The Joule heating flux density q is determined by the electric current density and electric field intensity,

$$q = \boldsymbol{J} \cdot \boldsymbol{E} = \sigma \cdot |\nabla \phi|^2 \tag{S2}$$

where, q is the Joule heat flux density, $\boldsymbol{J}$ the electric current density, $\boldsymbol{E}$ the electric field intensity, σ the conductivity of ITO film. ϕ the electric potential. ϕ satisfies $\nabla \cdot (\sigma \boldsymbol{E}) = -\sigma \nabla^2 \phi = 0$.

At the microheater's surface, the normal electric current density $\boldsymbol{J}_n$ is 0.

As for the other solid materials of the microchip, their temperature distributions satisfy the unsteady-state heat-conduction differential equation without internal heat source,

$$\rho_{gp} c_{gp} \frac{\partial T}{\partial t} = \nabla \cdot (k_{gp} \nabla T) \tag{S3}$$

where, ρ_{gp} is the density, c_{gp} the heat capacity, k_{gp} the thermal conductivity.

The heat transfer in fluids meets,

$$\rho_0 c_p \left(\frac{\partial T}{\partial t} + u \cdot \nabla T\right) - \nabla \cdot (k_f \nabla T) = 0 \tag{S4}$$

where, ρ_0 is the density, c_p the heat capacity, k_f the thermal conductivity.

At the interfaces of different materials, the temperature and the normal heat flux are continuous.

The chip surface-air satisfies,

$$-k\left(\frac{\partial T}{\partial n}\right)_s = h(T_s - T_r) \tag{S5}$$

where, k is the thermal conductivity, h the convective heat transfer coefficient, n the external normal line of the outer surface of the microchip, T_s the temperature of the chip's surface, T_r the temperature of the surrounding air.

2. Fluid convection.

The convection flow is governed by the Navier–Stokes and the continuity equations.

$$\rho_0(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = \mu(T)\nabla^2\boldsymbol{u} - \nabla p + \boldsymbol{F}_b + \boldsymbol{F}_c \tag{S6}$$

$$\nabla\cdot\boldsymbol{u} = 0 \tag{S7}$$

where, ρ_0 is the fluid density at room temperature T_0, $\mu(T)$ the dynamic viscosity at temperature T, p the pressure, $\boldsymbol{F}_b$ the buoyancy force, $\boldsymbol{F}_b = -\boldsymbol{g}[\rho_0 - \rho(T)] \approx -\boldsymbol{g}\rho_0\beta_T(T - T_0)$ ($\rho(T)$ the fluid density at temperature T, β_T the thermal expansion coefficient). $\boldsymbol{F}_c$ the thermo-capillary stress, $\boldsymbol{F}_c$=-$\sigma_T\nabla_S T$ (σ_T the temperature coefficient of surface tension, $\nabla_S T$ the tangential temperature gradient at fluidic interface).

At fluid-wall interfaces, the flow field meets the no-slip boundary condition: $\boldsymbol{u}_{wall} = 0$.

3. Particle migration.

The forces acting on microparticles include Stokes drag, gravity force, and thermophoretic force. The droplet velocity is

$$\boldsymbol{u}_d = \boldsymbol{u} + \boldsymbol{u}_G + \boldsymbol{u}_T \tag{S8}$$

where, $\boldsymbol{u}$ is the convection velocity, $\boldsymbol{u}_G$ the gravity velocity, $\boldsymbol{u}_T$the thermophoretic velocity.

Section S5: Numerical model and its boundary conditions

To numerically study the heat transfer and fluid convection characteristics of microfluidic device, we establish a 3D simulation model using a commercial Software of Comsol (COMSOL Multiphysics, 6.0). The numerical model contains three modules: electric current, heat transfer and fluid flow. For the boundary conditions, the fluid meets the non-slip boundary condition. At the solid-solid/ liquid-solid interfaces, the temperature and thermal flux are equal. At the chip-air interface, the thermal field meets the third kind of boundary (**Figure S6**). The boundary conditions and governing equations of the numerical model are shown in **Table S1**. The material parameters for simulation is shown in **Table S2**.

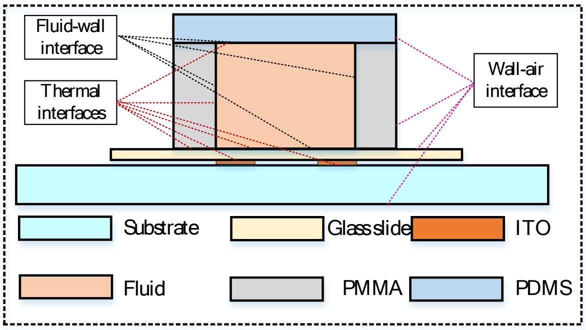

Figure S6. Side view of the microdevice.

Table S1. Governing equations and boundary conditions used in the numerical simulation.

Position	Electric field	Thermal field	Flow field
Microheaters	$\nabla\cdot(\sigma\boldsymbol{E}) = -\sigma\nabla^2\phi = 0$	$\rho_e c_e\frac{\partial T}{\partial t} = \nabla\cdot(k_e\nabla T) + \sigma\cdot\lvert\nabla\phi\rvert^2$	——
Surfaces of microheaters	$\boldsymbol{n}\cdot\nabla\phi = 0$	$\begin{cases} T_i = T_j \\ \Phi_i = \Phi_j \end{cases}$	——

Glass substrate and glass slide	——	$\rho_g c_g \frac{\partial T}{\partial t} = \nabla \cdot (k_g \nabla T)$	——
PMMA channel	——	$\rho_{pm} c_{pm} \frac{\partial T}{\partial t} = \nabla \cdot (k_{pm} \nabla T)$	——
PDMS cover	——	$\rho_{pd} c_{pd} \frac{\partial T}{\partial t} = \nabla \cdot (k_{pd} \nabla T)$	——
Fluids	——	$\rho_0 c_p (\frac{\partial T}{\partial t} + u \cdot \nabla T) - \nabla \cdot (k_f \nabla T) = 0$	$\begin{cases} \rho_0 (\boldsymbol{u} \cdot \nabla) \boldsymbol{u} = \mu(T) \nabla^2 \boldsymbol{u} - \nabla p + \boldsymbol{F}_b \\ \nabla \cdot \boldsymbol{u} = 0 \end{cases}$
Solid-solid interfaces	——	$\begin{cases} T_i = T_j \\ \Phi_i = \Phi_j \end{cases}$	——
Solid-liquid interfaces	——	$\begin{cases} T_i = T_j \\ \Phi_i = \Phi_j \end{cases}$	$\boldsymbol{u} = 0$
Wall-air	——	$-k(\frac{\partial T}{\partial n})_w = h(T_w - T_a)$	——

Notes: σ is the conductivity of the microheater; ϕ is the electric potential; ρ is the density; c is the heat capacity; k is the thermal conductivity; T_i and T_j are the temperatures of the two sides of the interfaces; Φ_i and Φ_j are the normal heat flux of the two sides of the interface; ρ_0 is the density of liquid media at room temperature; $\boldsymbol{u}$ is the velocity; $\mu(T)$ is the dynamic fluid viscosity at temperature T; p is the pressure; $\boldsymbol{F}_b = -\boldsymbol{g}(\rho_0 - \rho) \approx -\boldsymbol{g}\rho_0 \beta_T (T - T_0)$ is the buoyancy force.

Table S2. Material properties

	Electric conductivity [S/m]	Density [kg/m^3]	Heat capacity [J/(kg·K)]	Thermal conductivity [W/(m·K)]	Viscosity	Surface tension [mN/m]
Glass[1]	——	2203	703	1.38	——	——
PMMA[1]	——	1190	1420	0.19	——	——
Solid PDMS[1]	——	970	1460	0.16	——	——
Water[1]	——	$744.145+1.9447\times T-0.00368\times T^2$	$4035.841+0.492312\times T$	$-0.9004+0.0084\times T-1.1182\times 10^{-5}\times T^2$	$0.381-0.0044\times T+1.9\times 10^{-05}\times T^2-3.6736\times 10^{-08} T^3+2.6667\times 10^{-11}\times T^4$ [Pa·s]	$77.18-0.203\times(T-273.15)$
ITO[2]	2.1×10^5	7179	1000	2	——	——

Notes: T [K] is the temperature.

References:

[1] From the Material Library of Comsol software.
[2] Provided by the South China Science & Technology Company, China.