

Supplementary Information for

Magneto-Hyperdynamic Energetic Liquid Metals

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This PDF file includes:

Supplementary Modeling Note

Supplementary Figure S1 to S12

Other supplementary materials for this manuscript include the following:

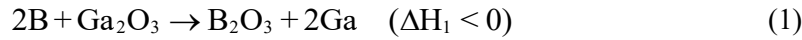
Supplementary Movies 1 to 7

Supplementary Note

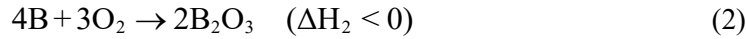
Simulation of displacement reaction of boron

Chemical Reaction Principles and Thermodynamic Models. The core of the simulation system is driven by two parts of chemical reactions: first, the heterogeneous reduction reaction between solid boron and liquid metal oxide Ga_2O_3 , namely the borothermal reduction reaction, which is used to generate reduced-state metallic gallium and destroy the original oxide barrier layer; second, the gas-liquid-solid composite oxidation reaction of boron and gallium components. A total of the following three core reaction pathways are considered within the system.

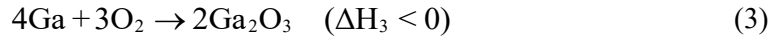
Main Borothermal Reduction Reaction, Reaction 1: After the system temperature crosses the in-situ ignition threshold, boron, acting as a strong reducing agent, undergoes a violent redox reaction with gallium oxide to produce liquid gallium, which possesses a heat transfer medium effect, and boron trioxide:



Macroscopic Oxidation Reaction of Solid Boron, Reaction 2: The direct exothermic oxidation reaction occurring when gas-phase oxygen molecules diffuse to the surface of highly active solid boron particles is one of the energy output sources of this reactor:



Oxidation Reaction of Liquid Gallium Metal, Reaction 3: The reduced highly active liquid metallic gallium or the metallic gallium component from the initial formulation reacts with oxygen to regenerate gallium oxide, and this reaction constitutes the closed-loop chemical cycle of gallium:



Chemical Reaction Principles and Thermodynamic Models. To accurately simulate the combustion characteristics of the reaction varying over time, a coupled system of ordinary differential equations containing 5 material component state variables and 1 temperature state variable was established.

Governing Equations and State Variables: The state vector of the system is defined as: $y = [n_{\text{B}}, n_{\text{Ga}_2\text{O}_3}, n_{\text{B}_2\text{O}_3}, n_{\text{Ga}}, n_{\text{O}_2}, T]^T$, where n_i represents the instantaneous number of moles (mol) of component i , and T is the absolute temperature of the system.

Kinetic Rate Equations and Ignition Penalty Function: The apparent chemical reaction rate r_i (mol/m³·s) of each reaction is determined by the Arrhenius law. Among them, for the main borothermal reduction reaction, a continuous adaptive ignition penalty function $f_{\text{ign}}(T)$ based on the Fermi-Dirac distribution form is introduced to characterize the physical limitation where the reaction is strongly inhibited due to capillary action and surface potential barriers at the heterogeneous interface of the solid before reaching the initial ignition temperature:

$$f_{\text{ign}}(T) = \frac{1}{1 + \exp\left(-\frac{T - T_{\text{ign}}}{\Delta T_{\text{ign}}}\right)} \quad (4)$$

When T is much smaller than T_{ign} , $f_{\text{ign}} \rightarrow 0$, and the reaction is strongly inhibited; after T crosses the ignition zone, $f_{\text{ign}} \rightarrow 1$, and the reduction reaction is fully activated.

Differential Equations for Material and Energy Conservation: According to the reaction stoichiometric ratios and energy balance, the final constructed system of differential equations for the reactor model is as follows:

$$r_1 = f_{\text{ign}}(T) \cdot A_1 \exp\left(-\frac{E_{a1}}{RT}\right) \sqrt{c_B c_{\text{Ga}_2\text{O}_3}} \quad (5)$$

$$r_2 = A_2 \exp\left(-\frac{E_{a2}}{RT}\right) \sqrt{c_B c_{\text{O}_2}} \quad (6)$$

$$r_3 = A_3 \exp\left(-\frac{E_{a3}}{RT}\right) \sqrt{c_{\text{Ga}} c_{\text{O}_2}} \quad (7)$$

Combining material conservation and system thermal balance, the system of differential equations is ultimately constructed as:

$$\frac{dn_B}{dt} = (-2r_1 - 4r_2)V, \quad \frac{dn_{\text{Ga}_2\text{O}_3}}{dt} = (-r_1 + 2r_3)V, \quad \frac{dn_{\text{B}_2\text{O}_3}}{dt} = (r_1 + 2r_2)V \quad (8)$$

$$\frac{dn_{\text{Ga}}}{dt} = (2r_1 - 4r_3)V, \quad \frac{dn_{\text{O}_2}}{dt} = (-3r_2 - 3r_3)V \quad (9)$$

$$\frac{dT}{dt} = \frac{Q_{\text{ext}} + Q_{\text{rxn}} - hA(T - T_{\text{inf}})}{m_{\text{Mix}} C_{p\text{Mix}}} \quad (10)$$

Wherein, the total exothermic power of the chemical reactions is:

$$Q_{\text{rxn}} = (-\Delta H_1 r_1 - \Delta H_2 r_2 - \Delta H_3 r_3) V \quad (11)$$

Calculation Process and Algorithmic Control. Because the chemical reaction time scale in millisecond level in the combustion system and the macroscopic heat dissipation/heating time scale in second level span several orders of magnitude, the system of differential equations exhibits extremely strong numerical stiffness. The simulation is advanced in MATLAB using the high-order variable-step stiff solver ode15s.

To prevent divergence caused by numerical integration oscillations during the violent thermal blowout phase, a zero-value truncation constraint was applied to the materials within the control kernel, and the physical suppression upper limit for the highest temperature was set to 3500 K.

Simulation Results Analysis and System Behavior Discussion. Through time-domain integral advancement, the system exhibited distinct transient thermal bifurcation characteristics.

Before reaching the ignition temperature, the system mainly relies on the external electrical heating power Q_{ext} to heat up slowly. Once the temperature crosses the 700 K threshold, the ignition function opens, and the reduction reaction and oxidation reaction intertwine with each other. The internal chemical heat generation of the system far exceeds the impact brought by the outside world, triggering a system thermal blowout, and the temperature increases to T_{max} .

The heat release curve presents a sharp single-peak structure. Through the logarithmic rate plot, it can be clearly seen that this peak originates from the explosive growth of Reaction 1 (borothermal reduction) after activation. Right after this process, the elemental liquid gallium participates in the oxidation cycle of Reaction 3, forming a kinetic autocatalytic effect. Along with the occurrence of the thermal blowout, the main reactants B and Ga_2O_3 exhibit a step-like plunge within an extremely short reaction window, which proves the high thermodynamic and kinetic feasibility of the borothermal reduction pathway mediated by liquid metallic gallium, and the passivation film on the solid boron surface is successfully destroyed to completely activate the reaction.

Simulation of skin effect

Geometric Simplification and 2D Axisymmetric Formulation. Since the composite target is a sphere and the surrounding 3-turn induction coil is aligned coaxially with the sphere's vertical axis of symmetry, the electromagnetic and thermal physical system possesses rotational symmetry. Consequently, the three-dimensional magneto-thermal coupling problem can be mathematically reduced to a two-dimensional axisymmetric formulation in the cylindrical coordinate system without any loss of physical fidelity. The modeling domain is thus simplified to a 2D meridian plane containing a semi-circular cross-section of the sphere and the adjacent coil domains.

Temperature-Dependent Conductivity. To incorporate the bidirectional coupling effect of temperature on the electromagnetic-thermal physics, the electrical resistivity $\rho_e(T)$ of the composite sphere is modeled using a linearized temperature dependence:

$$\rho_e(T) = \rho_0[1 + \alpha(T - T_{ref})]$$

$$\sigma(T) = \frac{1}{\rho_e(T)}$$

where $\rho_0 = 2.94 \times 10^{-7} \Omega \cdot \text{m}$ is the reference resistivity at the reference temperature $T_{ref} = 298 \text{ K}$, and $\alpha = 4 \times 10^{-4} \text{ K}^{-1}$ is the temperature coefficient of resistivity.

Transient Heat Transfer. The electromagnetic energy is converted into localized thermal energy via volumetric Joule heating Q_e . In cylindrical coordinates (r, ϕ, z) , the transient thermal behavior of the sphere is governed by:^[1]

$$\rho C_p \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(k_{iso} r \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left(k_{iso} \frac{\partial T}{\partial z} \right) + Q_e$$

$$Q_e = \frac{1}{2} \text{Re}(\mathbf{J}_{ind} \cdot \mathbf{E}^*) = \frac{1}{2} \sigma(T) |\mathbf{E}|^2$$

where $\rho = 6360 \text{ kg/m}^3$ is the density, $C_p = 380 \text{ J/(kg} \cdot \text{K)}$ is the constant pressure heat capacity, and $k_{iso} = 26.6 \text{ W/(m} \cdot \text{K)}$ is the thermal conductivity of the composite. $\mathbf{J}_{ind} = \sigma(T)\mathbf{E}$ and $\mathbf{E}$ denote the induced eddy current density and the induced electric field vector, respectively, with $\mathbf{E}^*$ being its complex conjugate.

Thermal Boundary Conditions. To capture the natural air convection and surface-to-ambient thermal radiation at the spherical boundary, the net heat flux at the interface is governed by:

$$-k_{iso} \nabla T \cdot \mathbf{n} = h(T - T_{ext}) + \varepsilon \sigma_{SB} (T^4 - T_{amb}^4)$$

where $h = 5 \text{ W/(m}^2 \cdot \text{K)}$ is the convective heat transfer coefficient representing natural air convection, $T_{ext} = 293.15 \text{ K}$ is the external temperature, $\varepsilon = 0.8$ is the surface emissivity of the sphere, $\sigma_{SB} \approx 5.67 \times 10^{-8} \text{ W/(m}^2 \cdot \text{K}^4)$ is the Stefan-Boltzmann constant, and $T_{amb} = 293.15 \text{ K}$ is the ambient reference temperature. $\mathbf{n}$ denotes the outward unit normal vector of the sphere surface.

Table S1. Comprehensive Parameters and Boundary Conditions Used in the Simulation

Parameter	Symbol	Value	Unit
Composite Radius	r_0	5	mm
Coil Turns	N	3	1
Coil Current	I_{coil}	240	A
Equivalent Relative Permeability ^[2]	μ_r	2.0	1
Mass Density	ρ	6360	kg/m ³
Heat Capacity	C_p	380	J/(kg · K)
Thermal Conductivity	k_{iso}	26.6	W/(m · K)
Reference Electrical Conductivity	σ_0	5.0×10^6	S/m
Reference Resistivity	ρ_0	2.94×10^{-7}	$\Omega \cdot m$
Temp. Coefficient of Resistivity	α	4.0×10^{-4}	K ⁻¹
Reference Temperature	T_{ref}	298	K
Convective Heat Transfer Coeff.	h	5	W/(m ² · K)
Surface Emissivity	ε	0.8	1
Ambient Reference Temperature	T_{amb}, T_{ext}	293.15	K

Figure S1

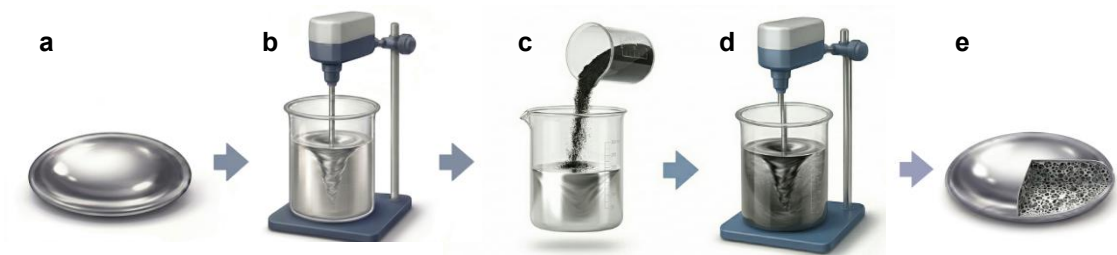


Figure S1. The preparation schematic illustration of MH-ELM. (a) Mixing gallium and indium in proportion. (b) Stirring pure gallium-indium alloy. (c) Adding magnetic powder. (d) Further stirring. (e) Obtaining MH-ELM.

Figure S2

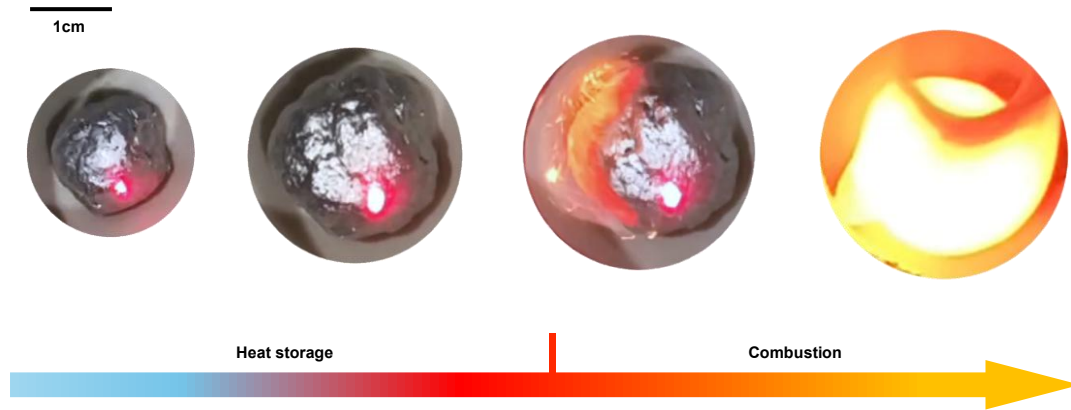


Figure S2. Hyperdynamic response of MH-ELM under alternating magnetic field actuation.

Figure S3

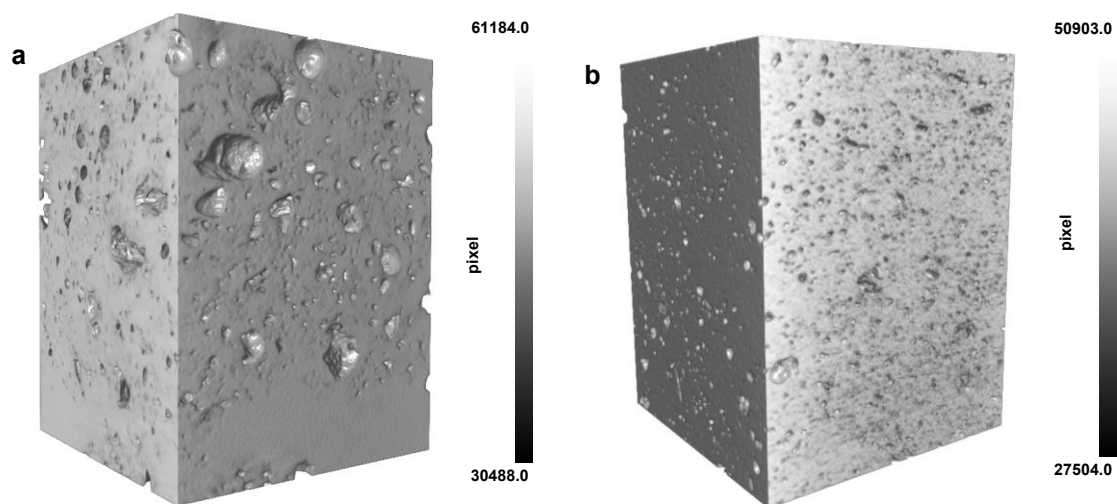


Figure S3. 3D X-ray microscopy of stirred liquid metals. (a) 3D Porosity of liquid metals after 1 h stirring. **(b)** 3D Porosity of liquid metals after 6 h stirring.

Figure S4

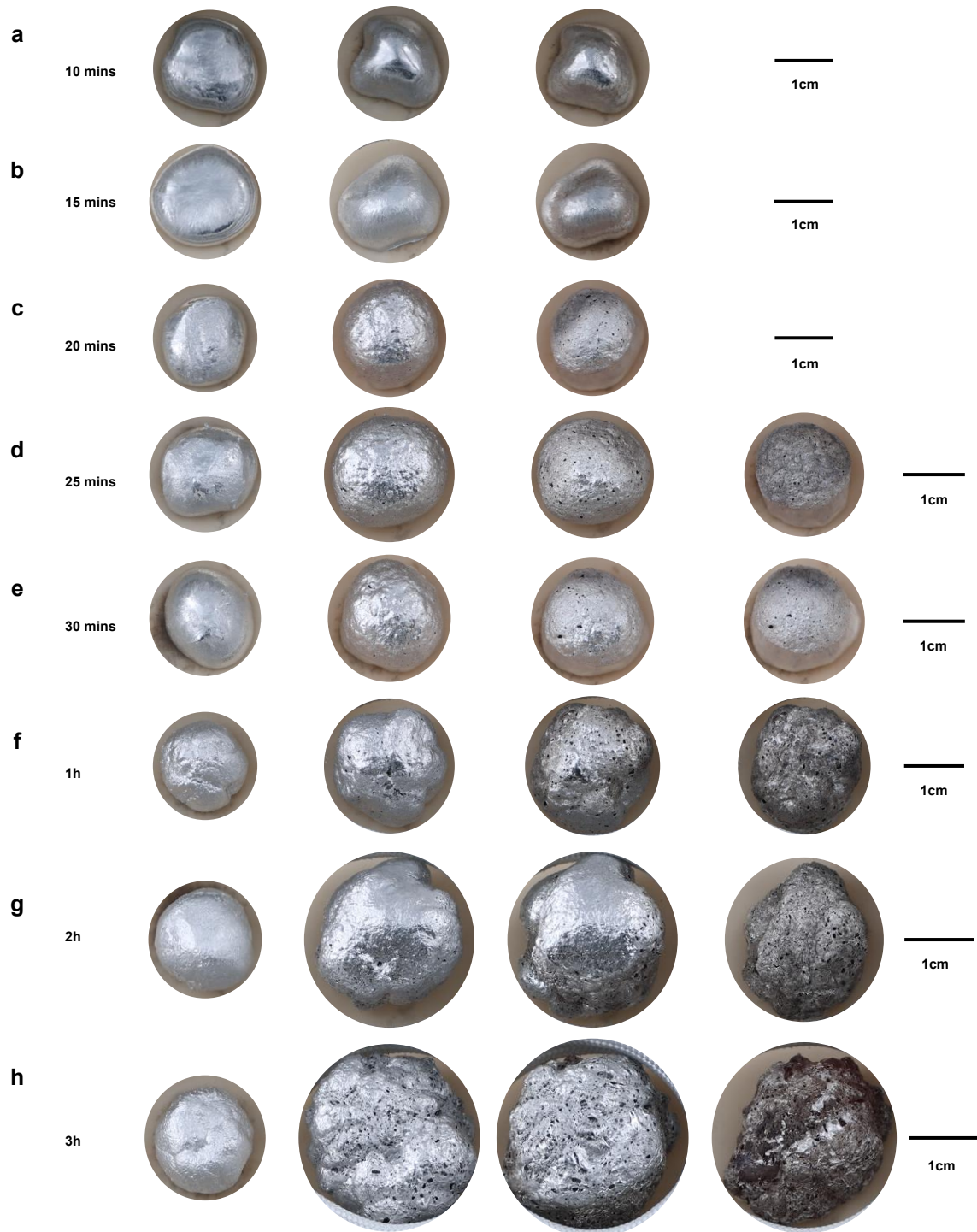


Figure S4 The response of stirred liquid metals under alternating magnetic field actuation.
(a-h) Alternating magnetic field actuation for liquid metals stirred by 10, 15, 20, 25, 30, 60, 120 and 180 mins, respectively.

Figure S5

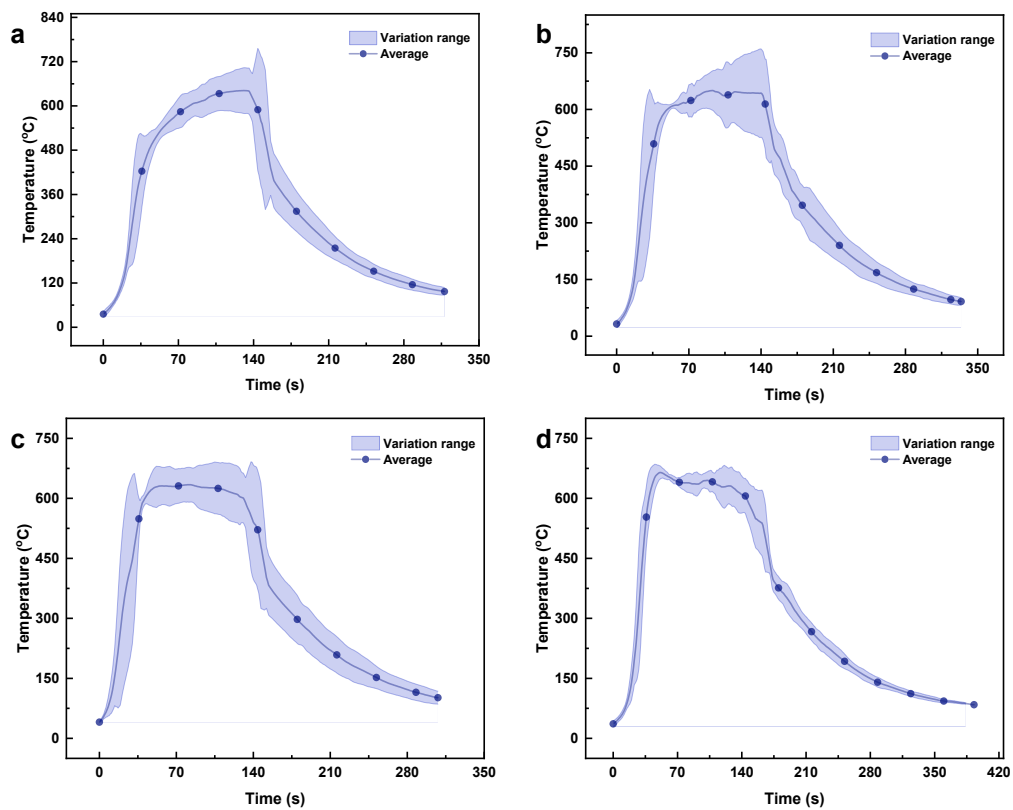


Figure S5. The temperature recording of Fe liquid metal system under alternating magnetic field actuation. (a-d) The temperature variation curves of 10wt%, 20wt%, 30wt%, 40wt% Fe liquid metal system, respectively.

Figure S6

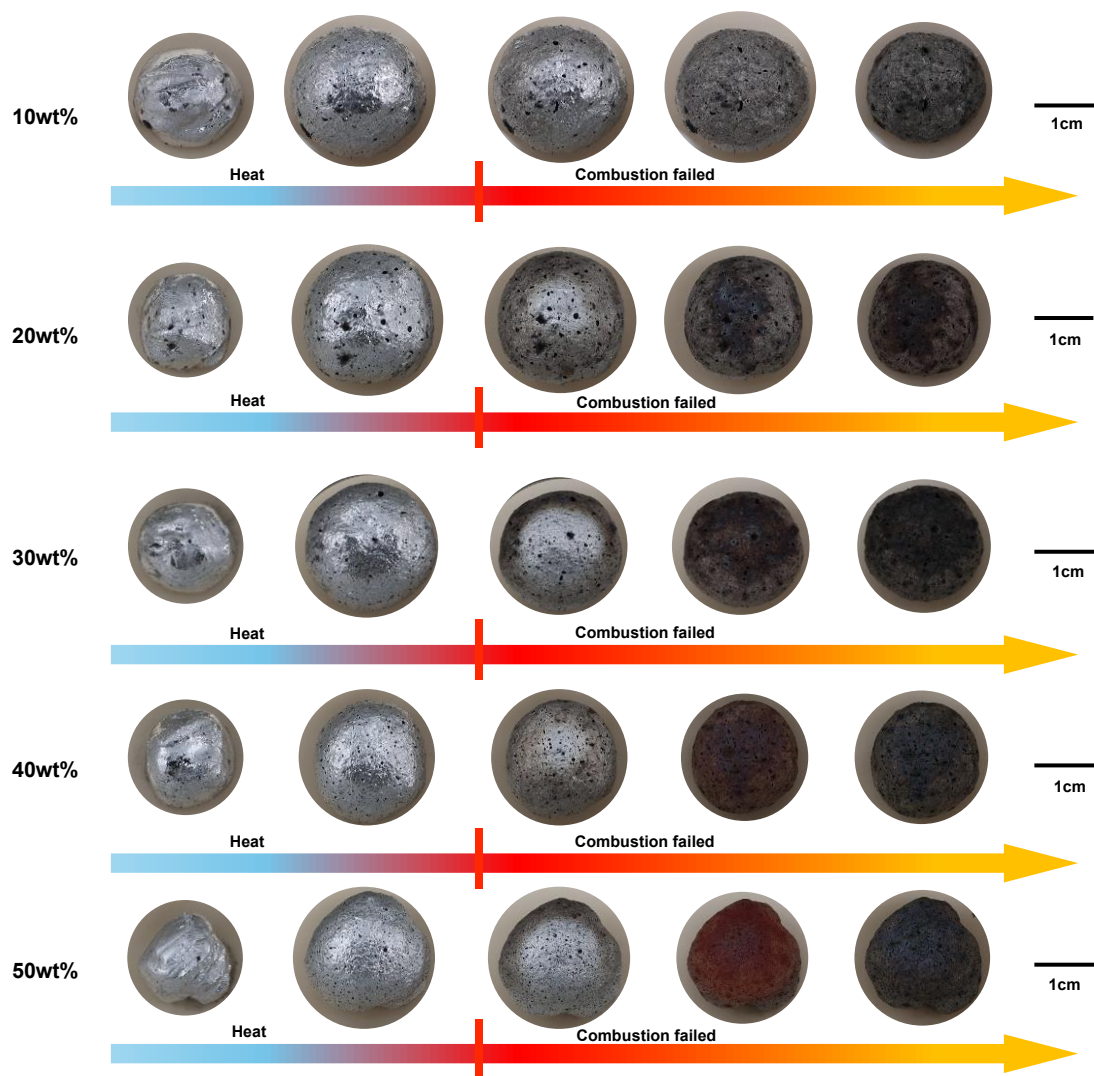


Figure S6. The response of Fe liquid metal system under alternating magnetic field actuation. The heat storage and failed combustion processes of 10wt%, 20wt%, 30wt%, 40wt%, 50wt% Fe liquid metal system, respectively.

Figure S7

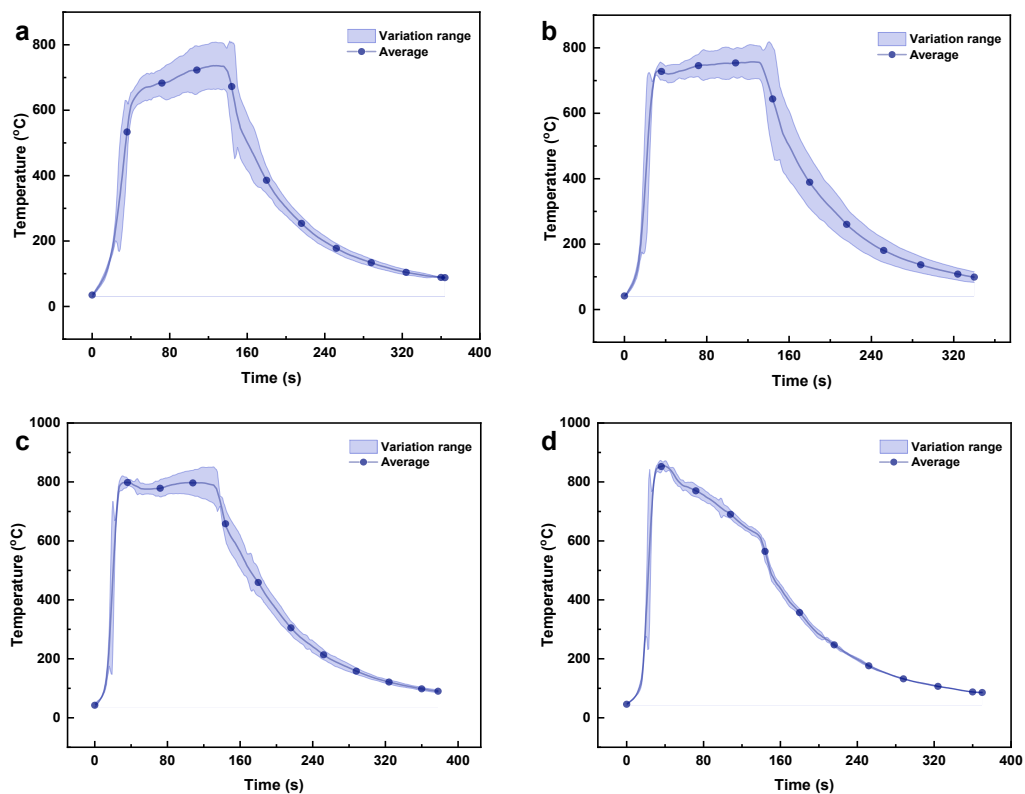


Figure S7. The temperature recording of NdFeB liquid metal system under alternating magnetic field actuation. (a-d) The temperature variation curves of 10wt%, 20wt%, 30wt%, 40wt% NdFeB liquid metal system, respectively.

Figure S8

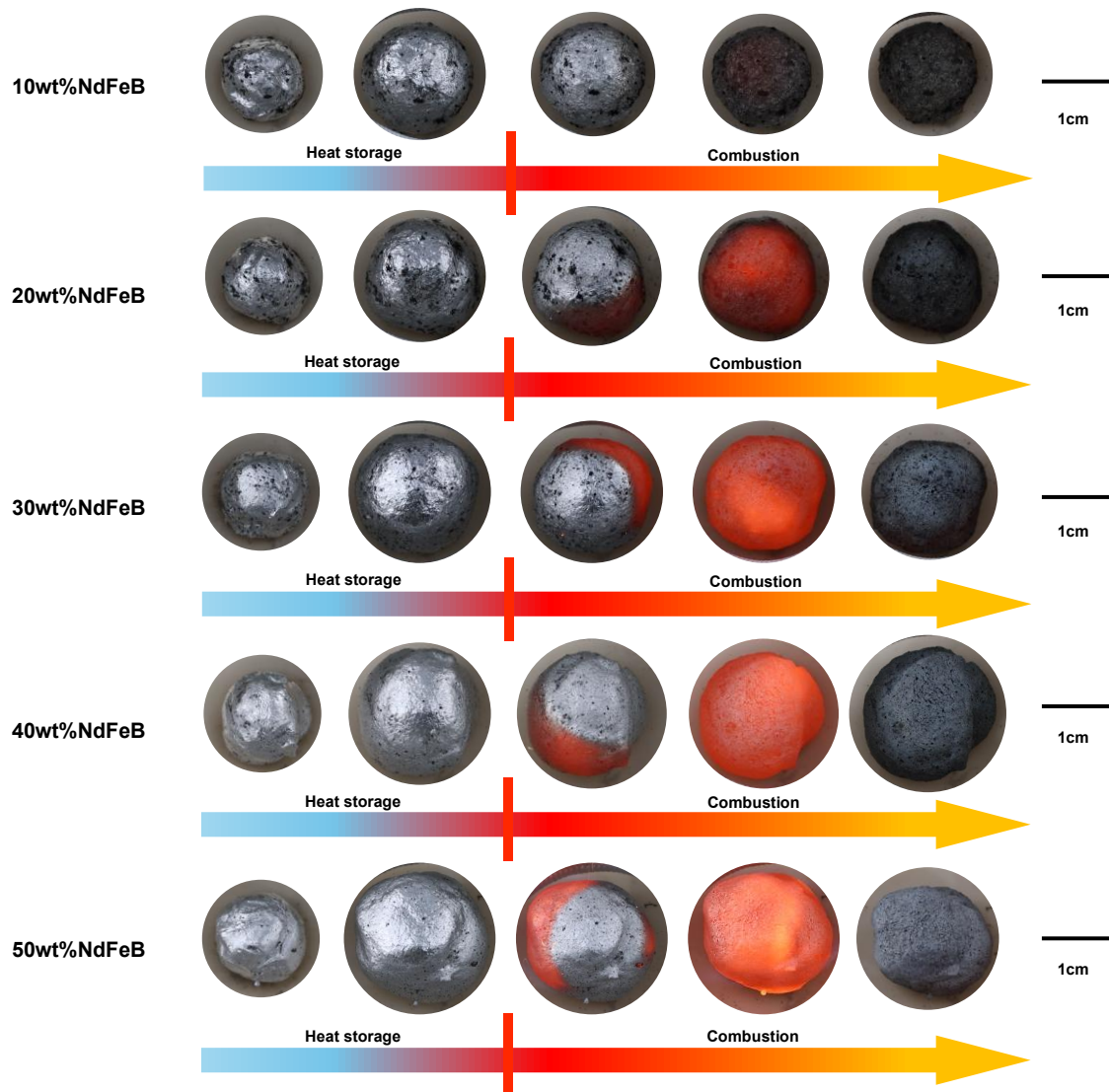


Figure S8. The response of NdFeB liquid metal system under alternating magnetic field actuation. The heat storage and combustion processes of 10wt%, 20wt%, 30wt%, 40wt%, 50wt% NdFeB liquid metal system, respectively.

Figure S9

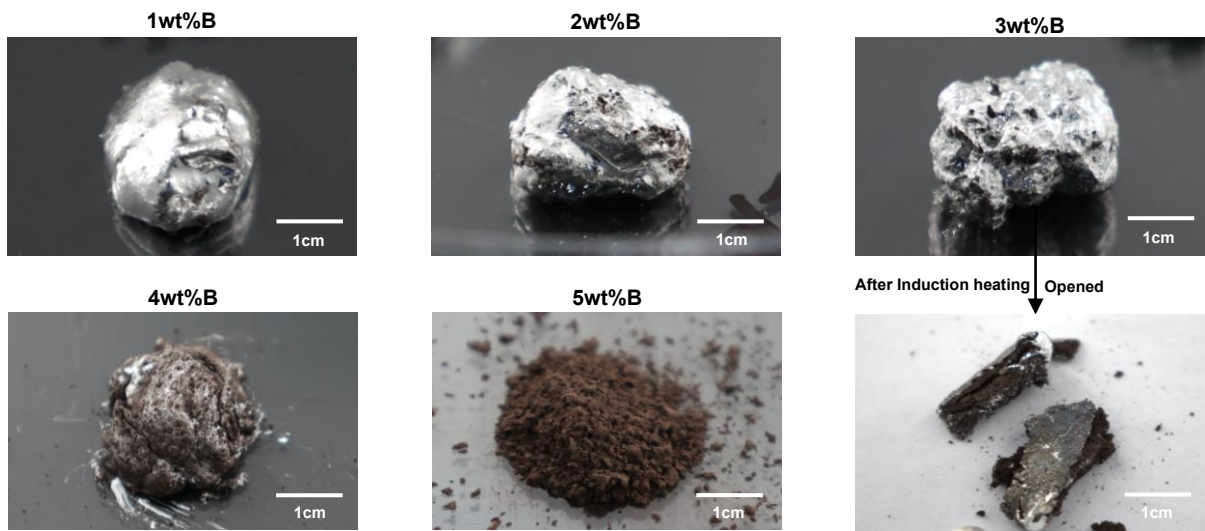


Figure S9. Liquid metals doped with different mass fractions of B particle. 1wt%B, 2wt%B, 3wt%B, 4wt%B, 5wt%B.

Figure S10

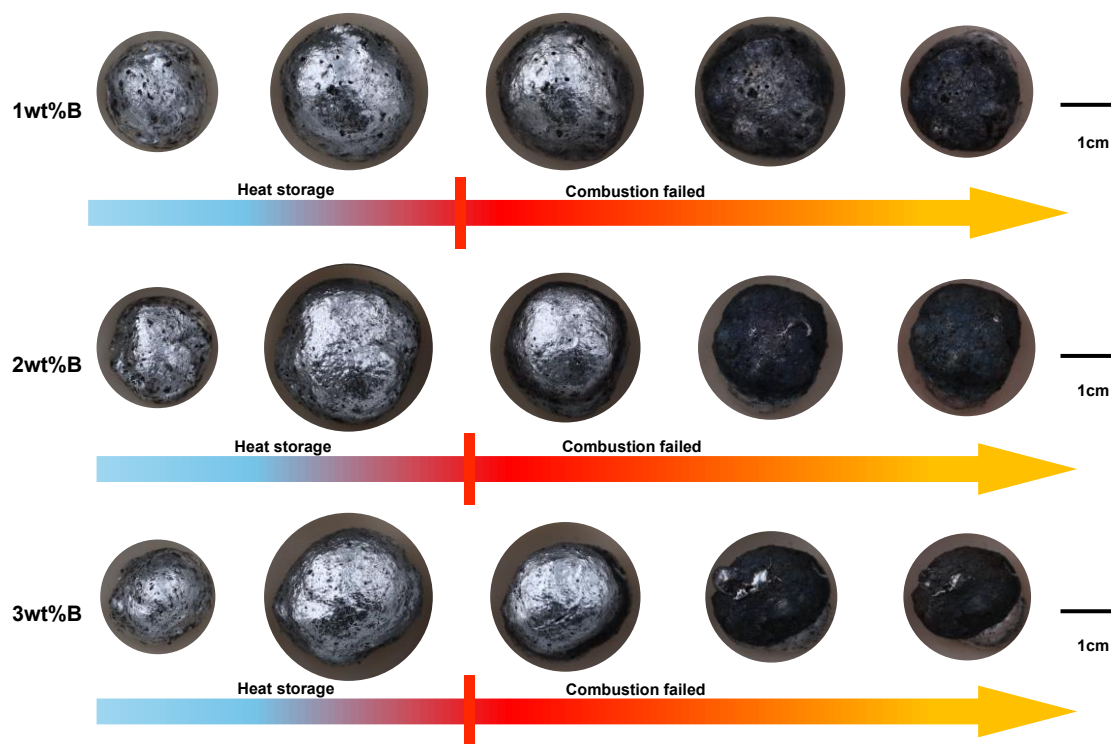


Figure S10. The response of B liquid metal system under alternating magnetic field actuation. The heat storage and combustion processes of 1wt%, 2wt%, 3wt% B liquid metal system, respectively.

Figure S11

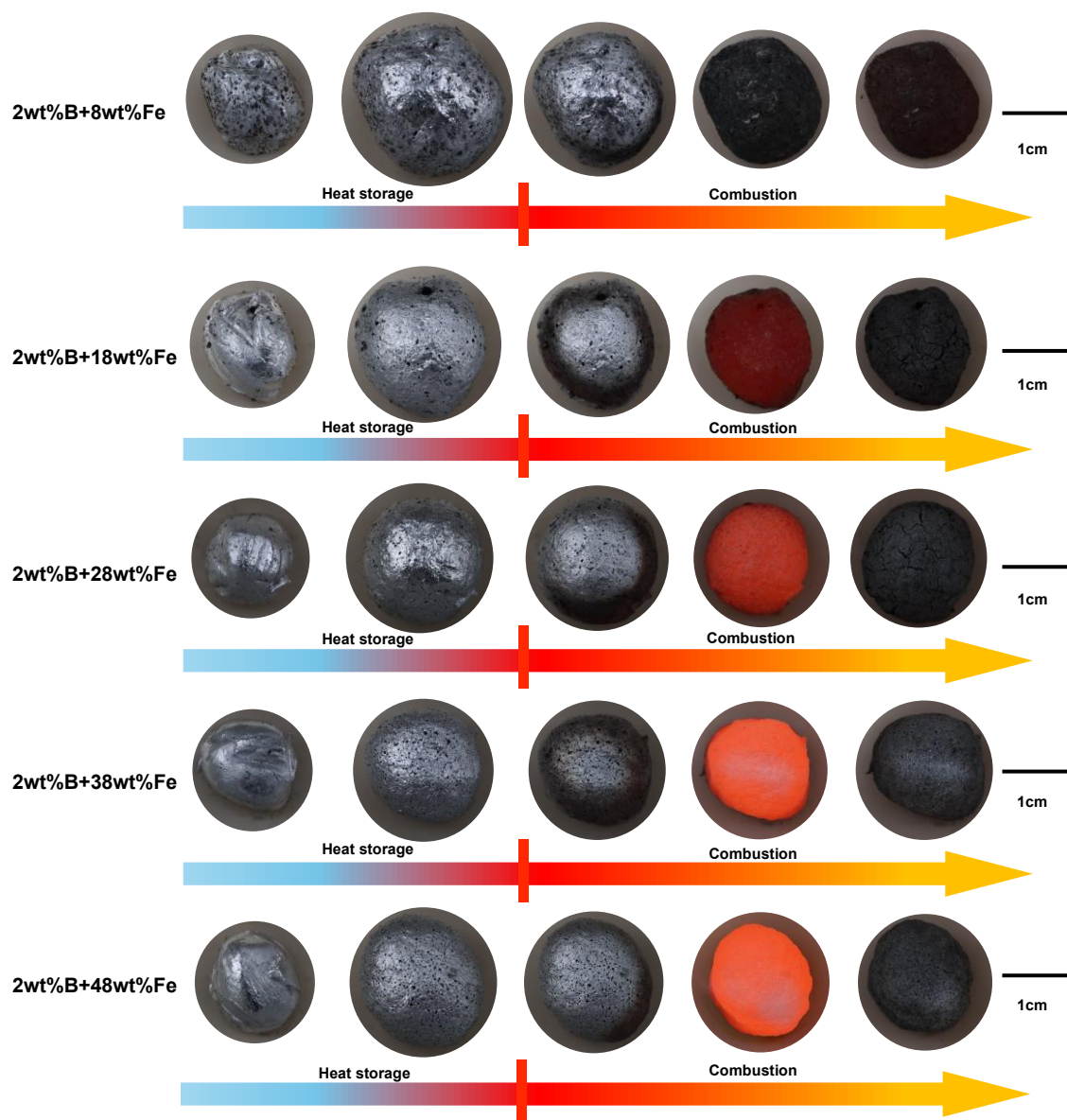


Figure S11. The response of B+Fe liquid metal system under alternating magnetic field actuation. The heat storage and combustion processes of 2wt%B+8wt%Fe, 2wt%B+18wt%Fe, 2wt%B+28wt%Fe, 2wt%B+38wt%Fe, 2wt%B+48wt%Fe liquid metal system, respectively.

Figure S12

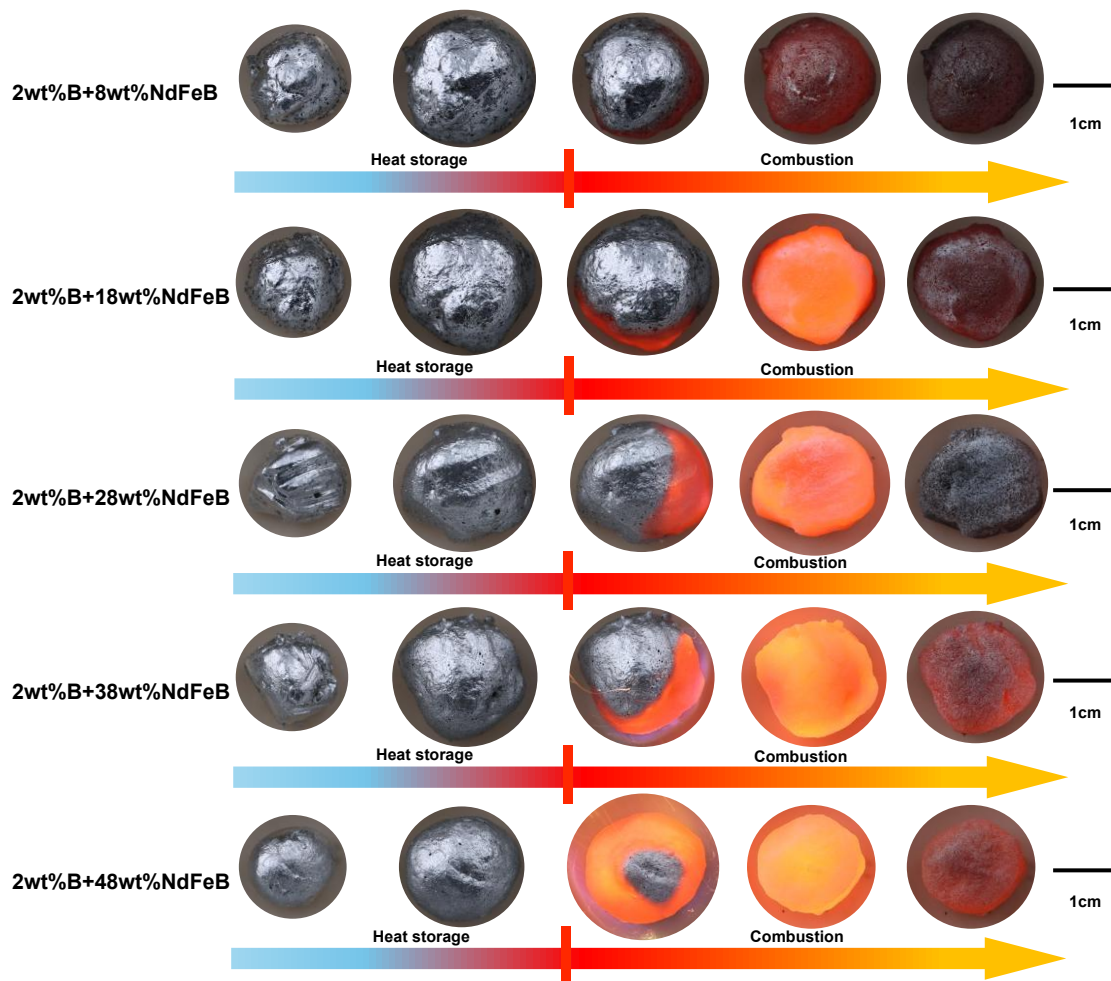


Figure S12. The response of B+NdFeB liquid metal system (MH-ELM) under alternating magnetic field actuation. The heat storage and combustion processes of 2wt%B+8wt%NdFeB, 2wt%B+18wt%NdFeB, 2wt%B+28wt%NdFeB, 2wt%B+38wt%NdFeB, 2wt%B+48wt%NdFeB liquid metal system, respectively.

Movie Legends

Movie S1. The hyperdynamic response of MH-ELM under AMF excitation.

Movie S2. The responses of pure liquid metals stirred for 10, 15, 20, 25. 30. 60. 120 and 180 mins under AMF actuation.

Movie S3. The responses of 10-50 wt% Fe liquid metal system under AMF actuation.

Movie S4. The responses of 10-50 wt% NdFeB liquid metal system under AMF actuation.

Movie S5. The responses of Fe+B liquid metal system under AMF actuation.

Movie S6. The responses of MH-ELM system under AMF actuation.

Movie S7. The high-speed camera recording the MH-ELM under AMF actuation.

Reference

1. Zhang, L.; Xiao, X.; Qi, H. Y.; Zhang, J. S.; Huang, Y. T., Nondestructive Determination of Young's Modulus of Interconnecting Thin Films by a Broadband Surface Acoustic Wave-Interdigital Transducer. *Phys. Status Solidi-Rapid Res. Lett.* **2023**, *17* (4), 10.
2. Wang, H. Y.; Liu, T. J.; Liu, S. F.; Jeng, J. L.; Guan, C. E., Thermal and Mechanical Properties of Stretched Recyclable Polyimide Film. *J. Appl. Polym. Sci.* **2011**, *122* (1), 210-219.