Supplementary Information (SI) for Nanoscale Advances.

Supplementary Information

Development of a laser induced graphene (LIG) and polylactic acid (PLA) shape memory composite with simultaneous multi-stimuli response and deformation self-sensing characteristics

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Steady-State Temperature Analysis During Resistive Joule Heating

One functionality of an integrated LIG pattern transferred onto a SMP substrate is its use as a resistive Joule heating element for electrically actuated shape recovery. However, several factors can affect the heating performance of the LIG pattern and the maximum achievable steady-state temperature in the SMP substrate. These key parameters include the applied voltage, electrical resistance of the LIG, the thermo-geometric properties of the SMP substrate (thermal conductivity and thickness), and the surrounding environment where the SMP/LIG composite is intended for use. Since the temperature and glass transition temperature (T_g) of the SMP are critical parameters in its applications, understanding how these factors affect the steady-state temperature of the SMP substrate becomes crucial. This knowledge allows for the design of LIG patterns that consider both the SMP properties and geometry for practical applications. This section explores the theoretical influence of these parameters on the achievable steady-state temperature. To achieve this, we will utilize two theoretical models, an analytical approach based on the equivalent thermal resistance circuit (ETRC) method and the finite element method (FEM).

ETRC models offer a straightforward tool for analyzing heat transfer in diverse scenarios due to their simplicity and computational efficiency [1,2]. It uses an analogy between electrical current and heat flux, employing fundamental Kirchhoff's Current Law (KCL) principles to solve heat transfer problems. This analytical model is built upon the following assumptions [3] :

- Steady-state heat transfer: Thermal conditions are constant over time.
- Heat is generated within the LIG at a uniform rate.
- Convective heat dissipation: Heat transfer to the surrounding environment occurs exclusively through convection with a constant heat transfer coefficient (h).
- Thermally isotropic substrate: The thermal properties SMP are considered uniform throughout.
- One-dimensional heat transfer: Heat dissipation through the thickness of the substrate is negligible.

Figure 1 shows a schematic of how heat transfer from LIG side to other side of SMP substrate. total heat generated by LIG ($q_{total} = V^2/R_e$) can be dissipated through LIG side (q_1) or the unheated side (q_2) after passing through SMP thickness (L). thus, equivalent thermal resistance circuit model can be drawn as shown in Figure 1. According to this thermal circuit, q_{total} can be calculated by eq. S1:

$$q_{total} = \frac{V^2}{R_e} = \frac{T_1 - T_{amb}}{R_{eq}} \qquad \text{(eq. S1)}$$

Where R_{eq} is the equivalent thermal resistant of the circuit and can be calculated using eq. S2:

$$R_{eq} = \left(\frac{1}{R_1 + R_3} + \frac{1}{R_2}\right)^{-1} \qquad \text{(eq. S2)}$$

Where R_1 is conductive thermal resistance of SMP substrate and R_2, and R_3 are convection resistances of LIG side surface and back side surface, respectively, and can be obtained using eq. S3.

$$R_1 = \frac{L}{kA_2}$$

$$R_2 = \frac{1}{hA_1} \qquad \text{(eq. S3)}$$

$$R_3 = \frac{1}{hA_2}$$

L, A_1, and k are thickness, area of back side of SMP/LIG composite, and the thermal conductive coefficient of SMP substrate. h is convection heat transfer coefficient of surrounding environment and A_2 is LIG surface area. q_2 also can be obtained using eq. S4:

$$q_2 = \frac{T_1 - T_2}{R_1} = \frac{T_2 - T_{amb}}{R_3} \qquad \text{(eq. S4)}$$

By combining eq. S1 eq. S2 and eq. S4 and some simplifications, temperature at unheated side SMP (T_2) can be obtained using eq. S5:

$$T_2 = \frac{R_1 T_{amb} + R_3 q_{total} R_{eq} + R_3 T_{amb}}{R_1 + R_3} \qquad \text{(eq. S5)}$$

eq. S5 directly governs the key parameters involved in Joule heating of an LIG pattern on top of an SMP substrate.

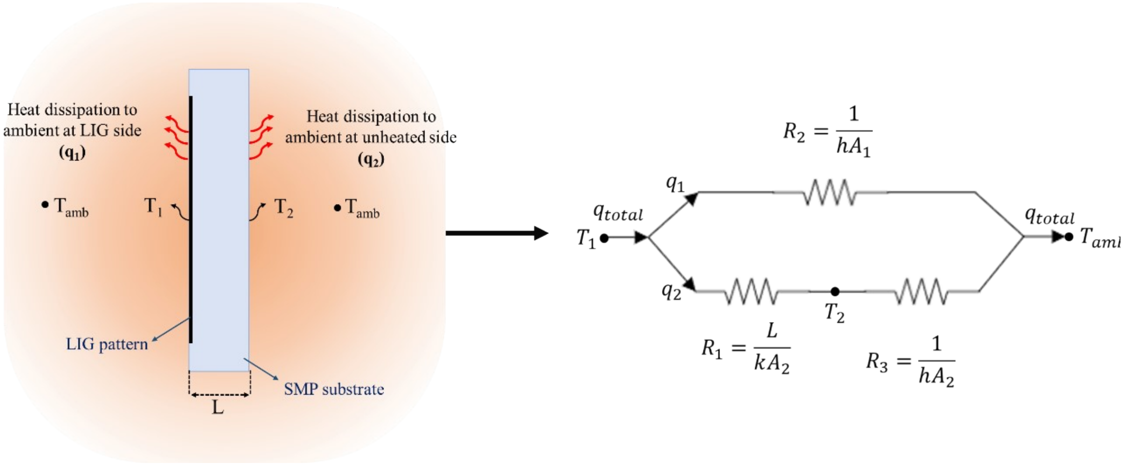

Figure 1. Schematic illustration of heat transfer from LIG side to SMP substrate and surrounding environment (left) and equivalent thermal resistance circuit model representing the heat transfer pathway (right).

In addition to the analytical model presented in eq. 5, the finite element method (FEM) was employed to simulate the Joule heating process and obtain the steady-state temperature distribution within the SMP/LIG specimen under varying electrical power input. The ANSYS software package and its electric-thermal module was utilized for these simulations.

The first step involved creating a three-dimensional (3D) model of the SMP/LIG specimen, replicating the exact dimensions of the real samples as depicted in Figure 2(a). A mesh size of 0.5 mm was chosen and the resulting mesh network is presented in Figure 2(b).

The LIG layer was assigned a thickness of 30 µm based on SEM image analysis. Considering this thickness and the results of sheet resistance measurements, an isotropic resistivity value of 0.1209 Ω·cm was assigned to the LIG pattern. The thermal conductivity (k) of PLA was assumed to be 0.183 $W \cdot m^{-1} \cdot K^{-1}$, as reported in the literature [4].

A heat convection boundary condition was applied to the model, assuming an ambient temperature of 25°C. The air free convection heat transfer coefficient (h) was set to 25 $W \cdot m^{-2} \cdot K^{-1}$. A voltage source was applied across the two ends of the LIG pattern to simulate electrical power input. The average steady-state temperature at the back surface of the specimen was recorded for various voltage levels.

Finally, the temperature values obtained from the FEM simulation and the analytical model (eq.5) were compared and validated against the experimental measurements.

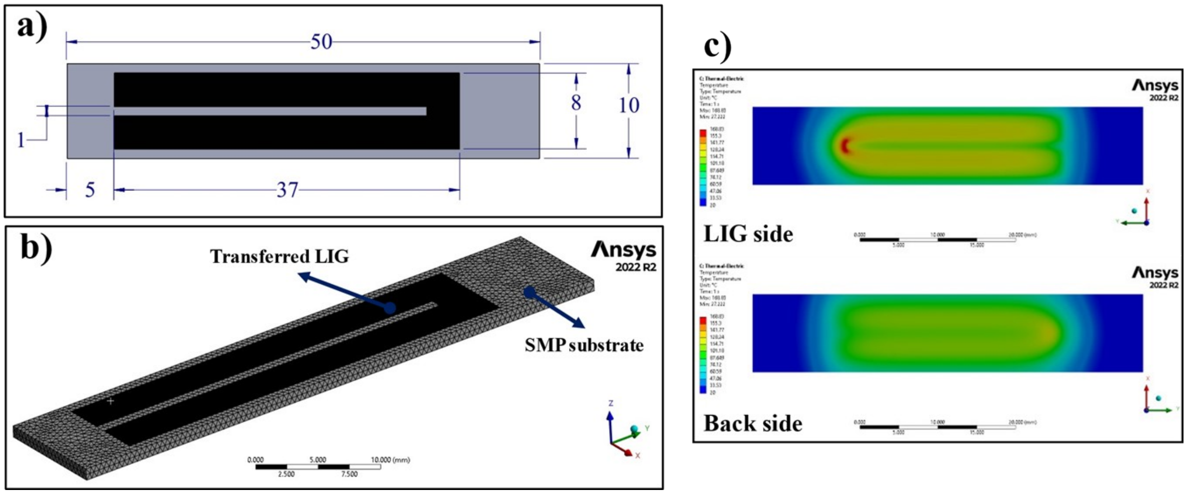

Figure 2. a) dimensions of SMP/LIG specimen. b) Generated mesh for FEM simulation. c) Typical temperature distribution at LIG and back side of SMP/LIG specimen for V=30 v

References

[1] S. Karagol, M. Bikdash, Generation of equivalent-circuit models from simulation data of a thermal system, IEEE Trans Power Electron 25 (2010) 820–828. https://doi.org/10.1109/TPEL.2009.2035317.

[2] B.H. Lee, K.S. Kim, J.W. Jung, J.P. Hong, Y.K. Kim, Temperature estimation of IPMSM using thermal equivalent circuit, IEEE Trans Magn 48 (2012) 2949–2952. https://doi.org/10.1109/TMAG.2012.2196503.

[3] J.P. Holman, Heat transfer., (2010).

[4] G. Spinelli, R. Kotsilkova, E. Ivanov, V. Georgiev, C. Naddeo, V. Romano, G. Spinelli, R. Kotsilkova, E. Ivanov, V. Georgiev, C. Naddeo, V. Romano, Thermal and Dielectric Properties of 3D Printed Parts Based on Polylactic Acid Filled with Carbon Nanostructures, Macromol Symp 405 (2022) 2100244. https://doi.org/10.1002/MASY.202100244.

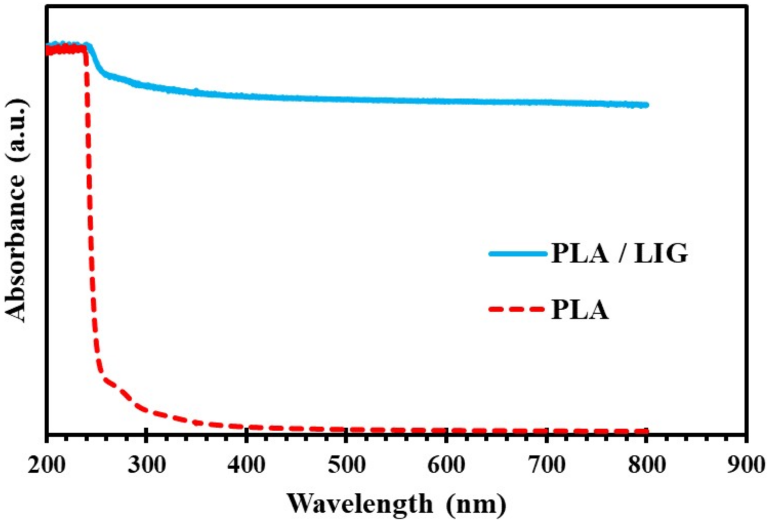

Figure S3. UV-VIS-NIR spectrum of PLA and LIG/PLA composite.