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Supporting Information for:

Optimized thermal design for excellent wearable thermoelectric generator

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1. Model building for finite element simulation

When a wearable thermoelectric generator (w-TEG) is worn on the wrist, the heat of human body flows from the blood core and passes through skin, bottom substrate, TE legs, top substrate and ambient environment in turn (Figure S1A). In order to ensure the accuracy of the simulation, the epidermis, dermis, and fat layer are considered in the skin model, as shown in Figure S1B. The corresponding parameter settings of the model for finite element simulation are listed in Table S1. Because the human skin surface is not absolutely flat, there is always a gap between the skin and the bottom substrate of w-TEG, which creates a relatively large contact thermal resistance, i.e., R_{contact}. It could be expressed as following:[1–3]

$$R_{contact} = \frac{(\sigma/m)}{1.25 \cdot A \cdot \kappa_s \cdot (P/H_c)^{0.95}} \tag{1}$$

where σ is the root mean square (RMS) of surface roughness and m is the average surface asperity slope, and A is the macroscopic contact area and κ_s is the harmonic mean thermal conductivity. P is the applied pressure and H_C is the microhardness of the substrate. The equivalent roughness (σ), surface slope (m) and thermal conductivity (κ_s) can be calculated from

$$\sigma = \sqrt{\sigma_{skin}^2 + \sigma_{sub}^2} \tag{2}$$

$$m = \sqrt{m_{skin}^2 + m_{sub}^2} \tag{3}$$

$$\kappa_s = \frac{2 \cdot \kappa_{skin} \cdot \kappa_{sub}}{\kappa_{skin} + \kappa_{sub}} \tag{4}$$

where σ_1, m_{skin} and κ_{skin} are the equivalent roughness, surface slope and thermal conductivity of skin, respectively. σ_{sub}, m_{sub} and κ_{skin} represent the equivalent roughness, surface slope and thermal conductivity of substrate, respectively.[4,5] The surface slope (m) can be estimated as a value depending on the surface roughness σ

$$m = 0.076 \cdot (\sigma \times 10^6)^{0.52} \tag{5}$$

2. Thermal Boundary Condition Settings

The widely used Pennes bio-heat equation describing heat transfer in the skin tissues is expressed as

$$Q = \rho_b \cdot C_{p,b} \cdot \omega_b(T_b - T) + Q_{met} \tag{6}$$

where ρ_b is the density of blood and $C_{p,\, b}$ is the Specific heat of blood, and ω_b is the blood perfusion rate and T_b is the arterial blood temperature. Q_{met} describes heat generation from metabolism. In addition, effects of blood transport are generally thought to exist only in the dermis layer and the epidermis layer could ignore the biological heat as a thermal resistance layer.[1–3,6–8]

According to Fourier's law, the heat transfer between w-TEG and the environment can be expressed as follow:

$$Q = h(T_{ambient} - T) \tag{7}$$

where h is the heat transfer coefficient and $T_{ambient}$ is the ambient temperature. The heat transfer coefficients of different positions of different materials of w-TEG are divided into three categories: the top surface, the bottom surface and the side surface of the horizontal plane, which are discussed separately. The heat transfer coefficient (h_{top}) at the top surface of the substrate and electrode can be calculated as:

$$h_{top} = \begin{cases} \frac{\kappa}{L} \cdot 0.54 Ra_L^{\frac{1}{4}} & if\ T > T_{ambient}\ and\ 10^4 \le Ra_L \le 10^7 \\ \frac{\kappa}{L} \cdot 0.15 Ra_L^{\frac{1}{3}} & if\ T < T_{ambient}\ and\ 10^7 \le Ra_L \le 10^{11} \\ \frac{\kappa}{L} \cdot 0.27 Ra_L^{\frac{1}{4}} & if\ T \le T_{ambient}\ and\ 10^5 \le Ra_L \le 10^{10} \end{cases} \tag{8}$$

Where κ is thermal conductivity of heat transfer medium (air), L is the characteristic length (defined as area / perimeter) and Ra_L is the rayleigh number .

The heat transfer coefficient (h_{bot}) at the bottom surface of the w-TEG can be calculated as:

$$h_{bot} = \begin{cases} \frac{\kappa}{L} \cdot 0.54 Ra_L^{\frac{1}{4}} & if\ T \le T_{ambient}\ and\ 10^4 \le Ra_L \le 10^7 \\ \frac{\kappa}{L} \cdot 0.15 Ra_L^{\frac{1}{3}} & if\ T \le T_{ambient}\ and\ 10^7 \le Ra_L \le 10^{11} \\ \frac{\kappa}{L} \cdot 0.27 Ra_L^{\frac{1}{4}} & if\ T > T_{ambient}\ and\ 10^5 \le Ra_L \le 10^{10} \end{cases} \tag{9}$$

Where κ is thermal conductivity of heat transfer medium (air), L is the characteristic length (defined as area / perimeter) and Ra_L is the rayleigh number. The heat transfer coefficient (h_{bot}) at the side surface of the w-TEG can be calculated as:

$$h_{side} = \begin{cases} \frac{\kappa}{H}\left(0.68 + \frac{0.67 Ra_L^{1/4}}{\left(1+\left(\frac{0.492}{\mu C_p}\right)^{4/9}\right)}\right) & if\ Ra_L \le 10^9 \\ \frac{\kappa}{H}\left(0.825 + \frac{0.387 Ra_L^{1/6}}{\left(1+\left(\frac{0.492}{\mu C_p}\right)^{8/27}\right)}\right) & if\ Ra_L > 10^9 \end{cases} \tag{10}$$

Where κ, μ, C_p are thermal conductivity of heat transfer medium (air), dynamic viscosity and heat capacity of air at the qualitative temperature (T_q) respectively. The qualitative temperature is defined as ($T_{\text{side}} + T_{\text{ambient}}$)/2, where T_{side} is the temperature of the side surface of the w-TEG. Ra represents the Rayleigh number defined by T_q and the characteristic length H (the side height of the cube).

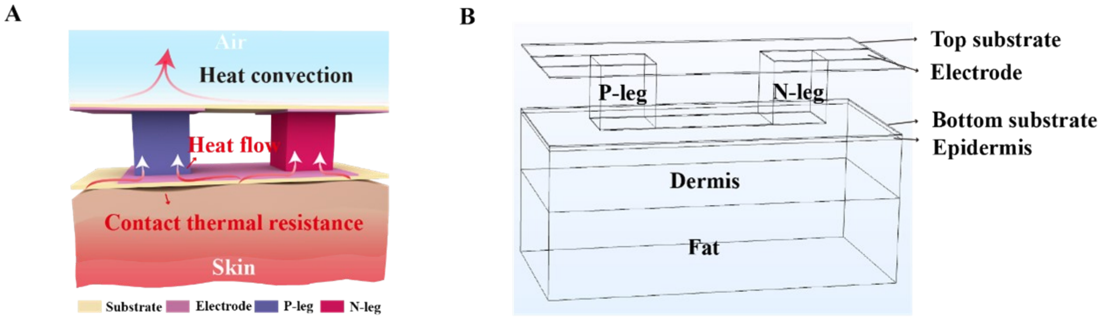
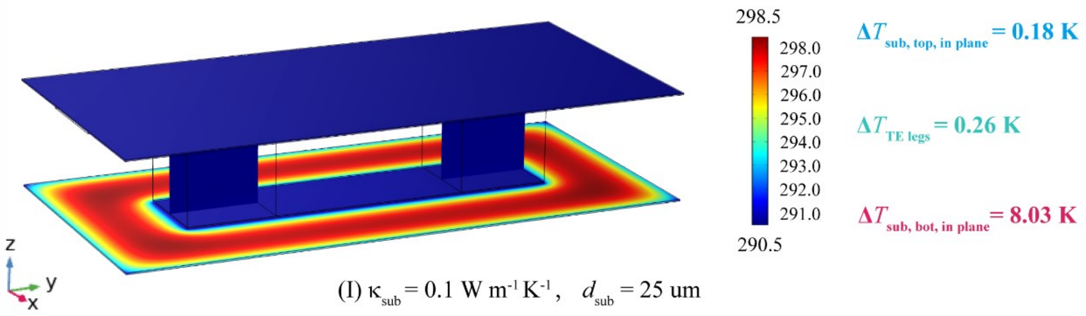


Figure S1. (A) Schematic diagram of the simulation model, (B) Actual simulation model for finite element analysis (FEA) by COMSOL

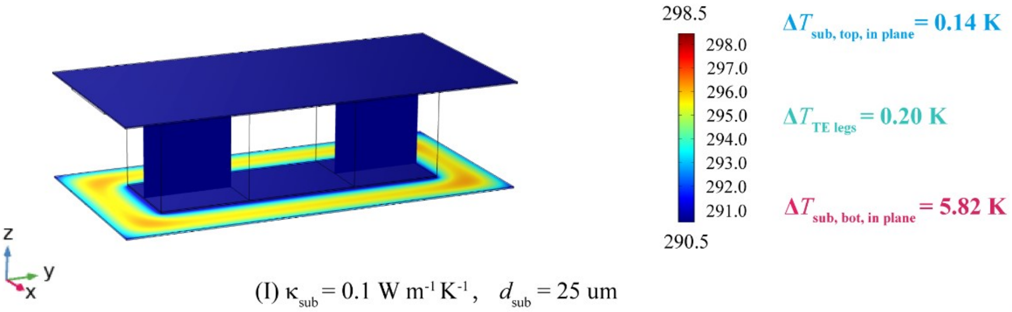
Table S1 Parameter settings of the model for finite element simulation

Material	Height (mm)	Parameter	Value
TE legs	1.6	TE properties	In Fig. S7
Copper electrode	0.02	Resistivity (S m^{-1})	7000000
		Thermal conductivity (W m^{-1} K^{-1})	400
Substrate	Variable	Thermal conductivity (W m^{-1} K^{-1})	Variable
Epidermis	0.1	Thermal conductivity (W m^{-1} K^{-1})	0.235
		Surface roughness (μm)	21.69
		Surface asperity slope (rad)	0.3
		Microhardness (MPa)	0.1225
		Contact pressure (kPa)	0.5
Dermis	1.5	Thermal conductivity (W m^{-1} K^{-1})	0.445
		Blood perfusion rate (s^{-1})	0.03
		Density × specific heat of blood (10^6 J m^{-3} K)	4.218
Fat	4.4	Body core temperature T_{core} (K)	310
		Thermal conductivity (W m^{-1} K^{-1})	0.185
		Metabolic heat generation (W m^{-3})	368

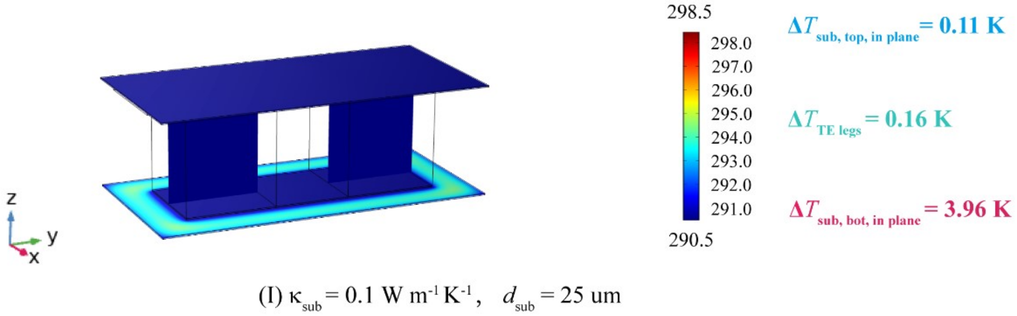
A. FF = 10 %



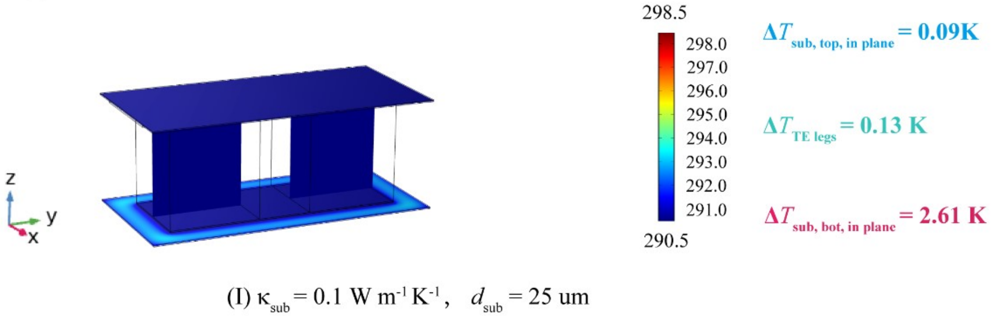
B. FF = 20 %



C. FF = 30 %



D. FF = 40 %



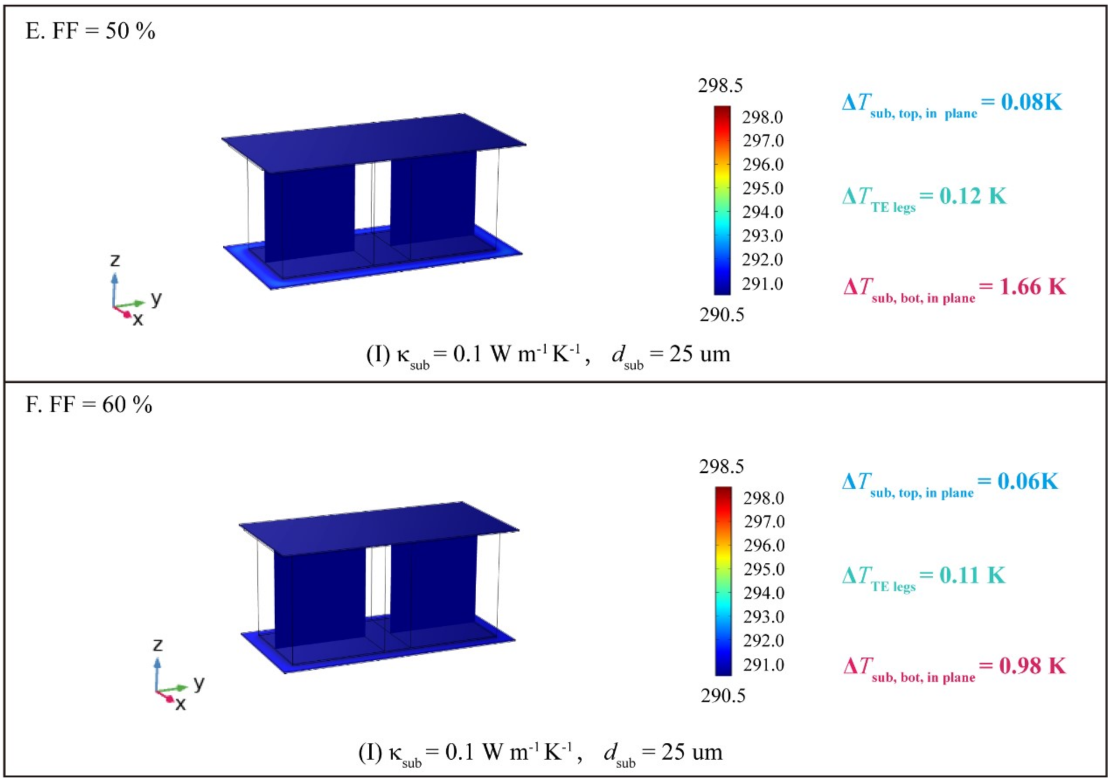
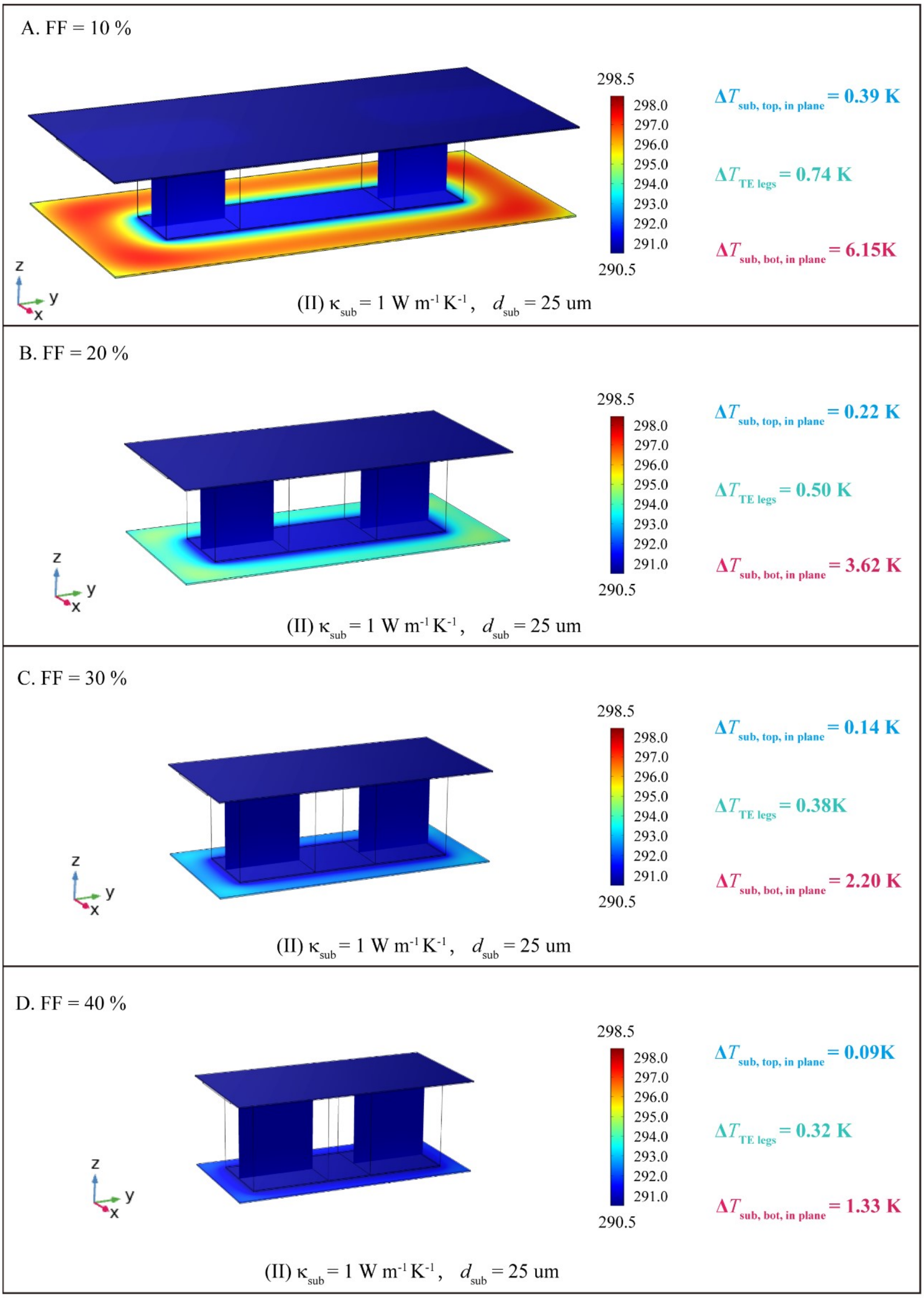


Figure S2. Temperature distribution of bottom substrate, thermoelectric legs and top substrate in the w-TEG with different fill factors (FFs): (A) FF = 10 %, (B) FF = 20 %, (C) FF = 30 %, (D) FF = 40%, (E) FF = 50%, (F) FF = 60%. Note: the thermal conductivity of the substrate (κ_{sub}) is 0.1 W m^{-1} K^{-1}, and the thickness of substrate (d_{sub}) is 25 µm.


A. FF = 10 %
298.5
298.0
297.0
296.0
295.0
294.0
293.0
292.0
291.0
290.5
$\Delta T_{\text{sub, top, in plane}}$ = 0.39 K
$\Delta T_{\text{TE legs}}$ = 0.74 K
$\Delta T_{\text{sub, bot, in plane}}$ = 6.15K
z
y
x
(II) κ_{sub} = 1 W m^{-1} K^{-1}, d_{sub} = 25 um
B. FF = 20 %
298.5
298.0
297.0
296.0
295.0
294.0
293.0
292.0
291.0
290.5
$\Delta T_{\text{sub, top, in plane}}$ = 0.22 K
$\Delta T_{\text{TE legs}}$ = 0.50 K
$\Delta T_{\text{sub, bot, in plane}}$ = 3.62 K
z
y
x
(II) κ_{sub} = 1 W m^{-1} K^{-1}, d_{sub} = 25 um
C. FF = 30 %
298.5
298.0
297.0
296.0
295.0
294.0
293.0
292.0
291.0
290.5
$\Delta T_{\text{sub, top, in plane}}$ = 0.14 K
$\Delta T_{\text{TE legs}}$ = 0.38K
$\Delta T_{\text{sub, bot, in plane}}$ = 2.20 K
z
y
x
(II) κ_{sub} = 1 W m^{-1} K^{-1}, d_{sub} = 25 um
D. FF = 40 %
298.5
298.0
297.0
296.0
295.0
294.0
293.0
292.0
291.0
290.5
$\Delta T_{\text{sub, top, in plane}}$ = 0.09K
$\Delta T_{\text{TE legs}}$ = 0.32 K
$\Delta T_{\text{sub, bot, in plane}}$ = 1.33 K
z
y
x
(II) κ_{sub} = 1 W m^{-1} K^{-1}, d_{sub} = 25 um

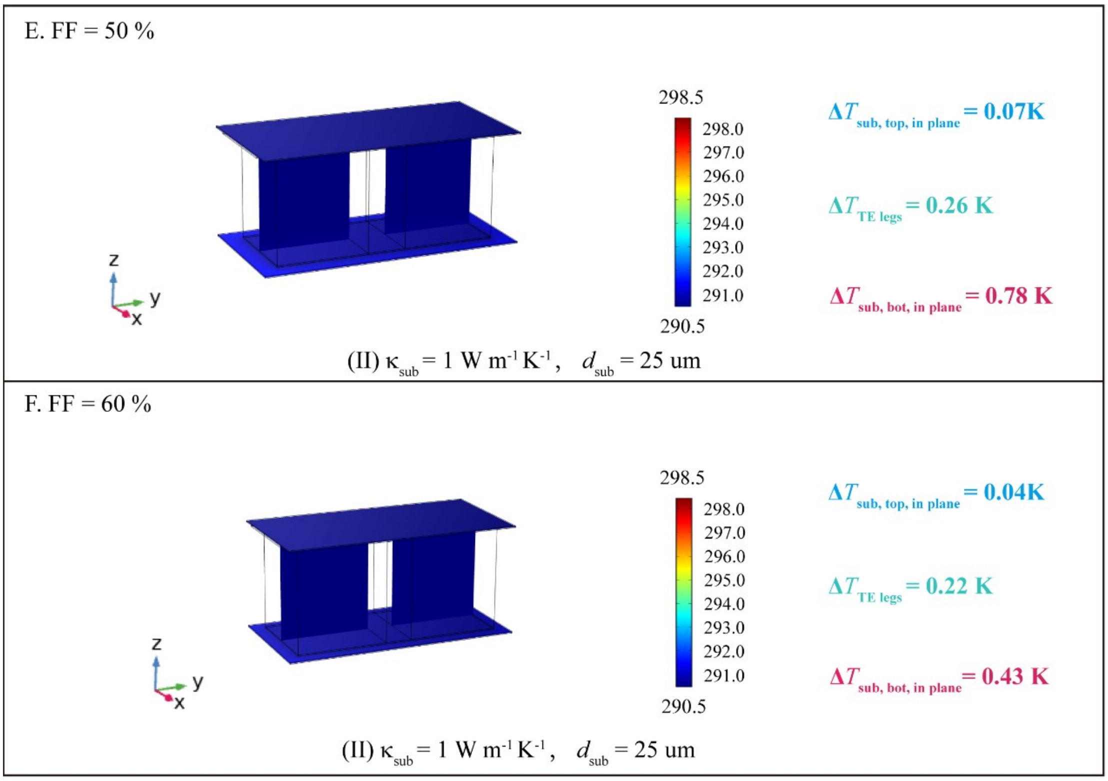
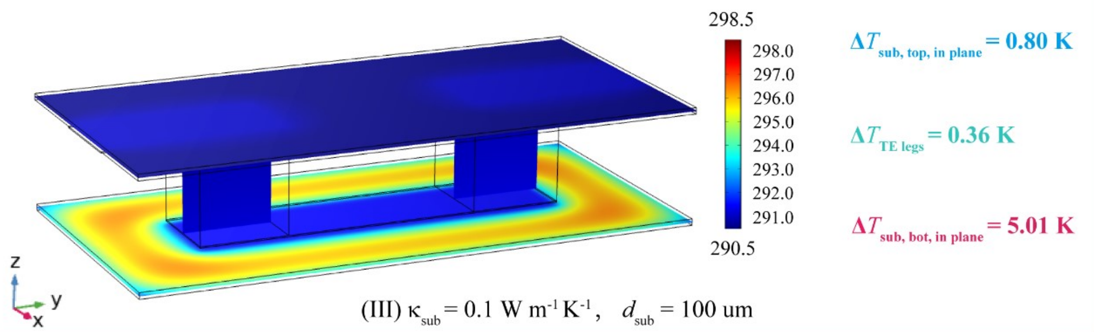
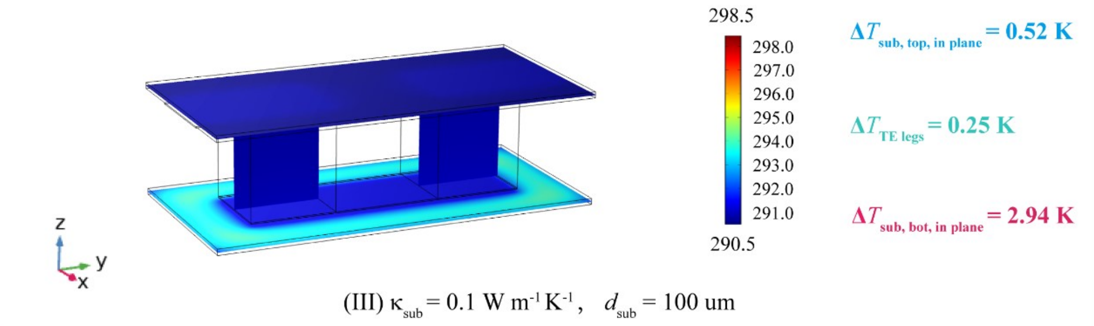


Figure S3. Temperature distribution of bottom substrate, thermoelectric legs and top substrate in the w-TEG with different fill factors (FFs): (A) FF = 10 %, (B) FF = 20 %, (C) FF = 30 %, (D) FF = 40%, (E) FF = 50%, (F) FF = 60%. Note: the thermal conductivity of the substrate (κ_{sub}) is 1 W m^{-1} K^{-1}, and the thickness of substrate (d_{sub}) is 25 μm.

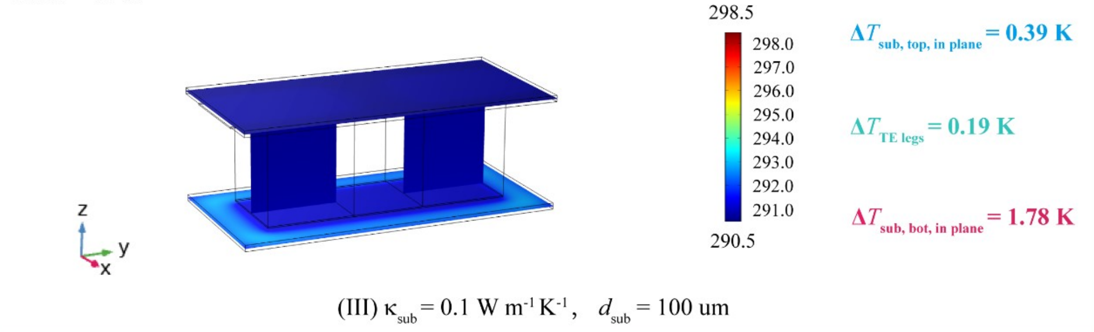
A. FF = 10 %



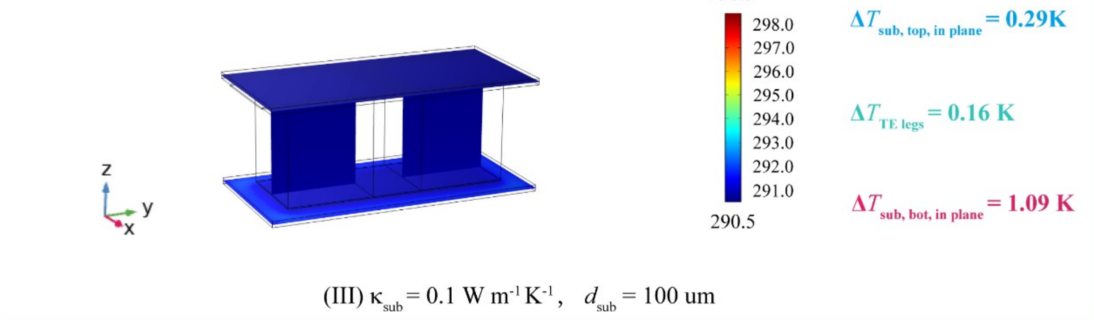
B. FF = 20 %



C. FF = 30 %



D. FF = 40 %



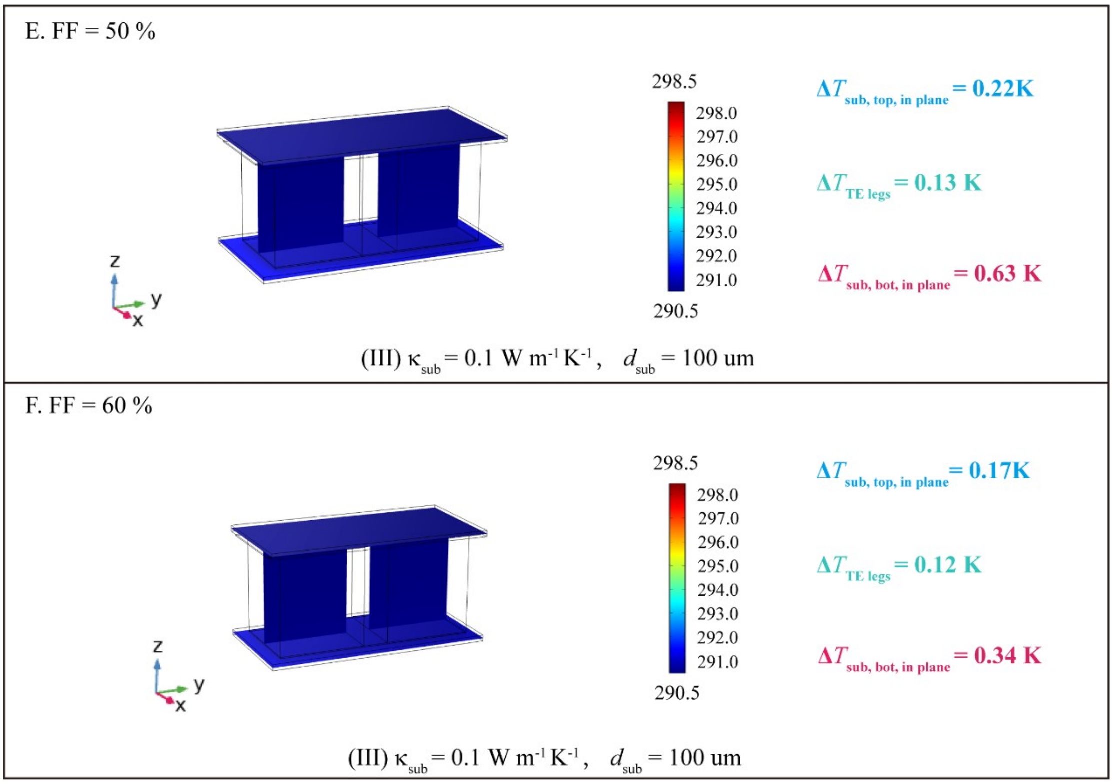


Figure S4. Temperature distribution of bottom substrate, thermoelectric legs and top substrate in the w-TEG with different fill factors (FFs): (A) FF = 10 %, (B) FF = 20 %, (C) FF = 30 %, (D) FF = 40%, (E) FF = 50%, (F) FF = 60%. Note: the thermal conductivity of the substrate (κ_{sub}) is 0.1 W m^{-1} K^{-1}, and the thickness of substrate (d_{sub}) is 100 μm.

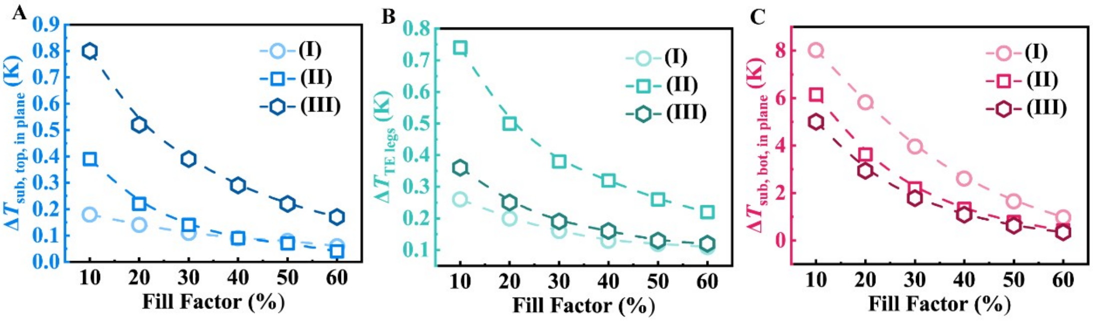


Figure S5. Temperature distribution of bottom substrate, thermoelectric legs and top substrate in the w-TEG with different fill factors (FFs): (A) FF = 10 %, (B) FF = 20 %, (C) FF = 30 %, (D) FF = 40%, (E) FF = 50%, (F) FF = 60%. Note: (I) the thermal conductivity of the substrate (κ_{sub}) is 0.1 W m^{-1} K^{-1}, and the thickness of substrate (d_{sub}) is 25 μm.(II) the thermal conductivity of the substrate (κ_{sub}) is 1 W m^{-1} K^{-1}, and the thickness of substrate (d_{sub}) is 25 μm. (III) the thermal conductivity of the substrate (κ_{sub}) is 0.1 W m^{-1} K^{-1}, and the thickness of substrate (d_{sub}) is 100 μm.

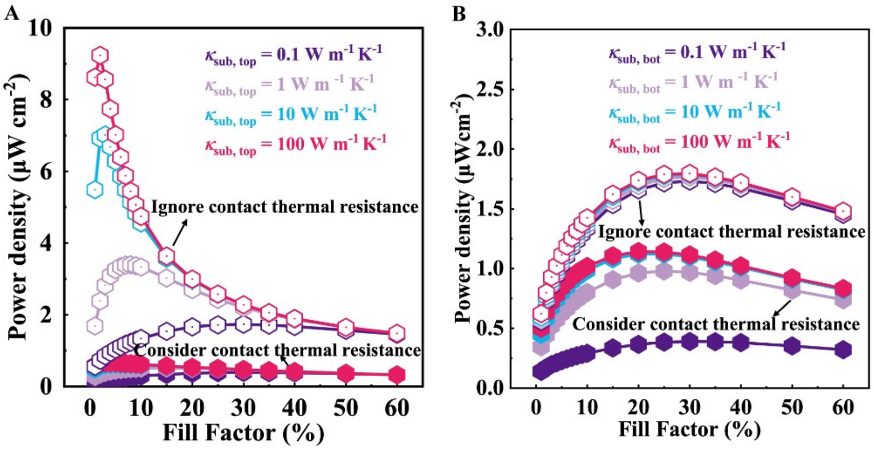


Figure S6. Comparing the effects on the relationship among FF, κ and power density when considering and ignoring the contact thermal resistance between the skin and the w-TEG interface. (A) When the thermal conductivity of the bottom substrate ($\kappa_{sub, bot}$) is 0.1 W m^{-1} K^{-1}, and the thermal conductivity of the top substrate ($\kappa_{sub, top}$) is 0.1, 1, 10, and 100 W m^{-1} K^{-1}, respectively. (B) When $\kappa_{sub, top}$ = 0.1 W m^{-1} K^{-1}, and $\kappa_{sub, bot}$ is 0.1, 1, 10, and 100 W m^{-1} K^{-1}, respectively.

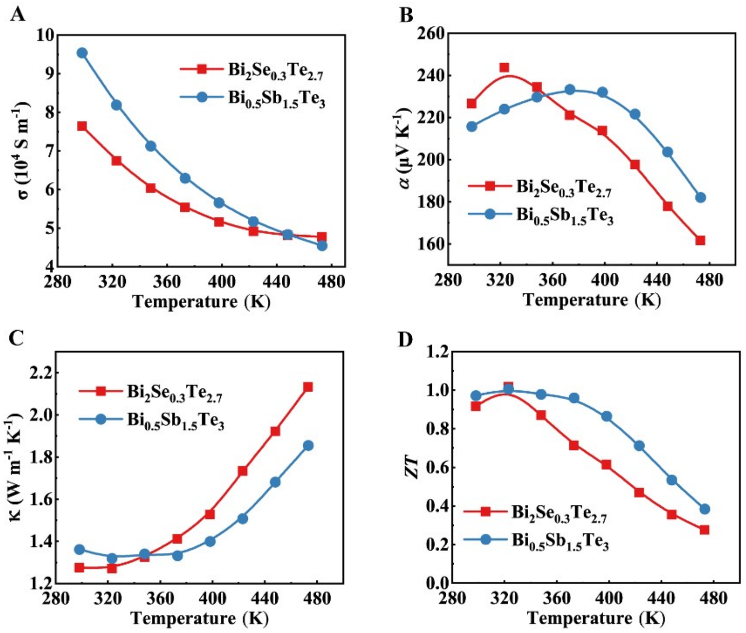


Figure S7. TE properties of the P/N-type TE legs material used for simulation and fabrication of the w-TEGs in this paper.

Table S2 Weights of w-TEGs with PI substrate and laminated substrate with different fill factor.

FF (%)	Weight(g)	
	w-TEGs with PI substrate	w-TEGs with laminated substrate
10	0.93	1.01
20	1.62	1.71
30	2.50	2.59
40	3.05	3.17

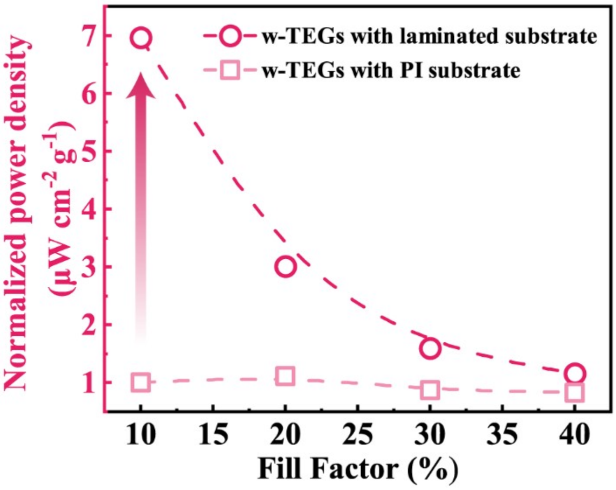


Figure S8. Normalized power density for w-TEGs with PI substrate and laminated substrate with different fill factor.

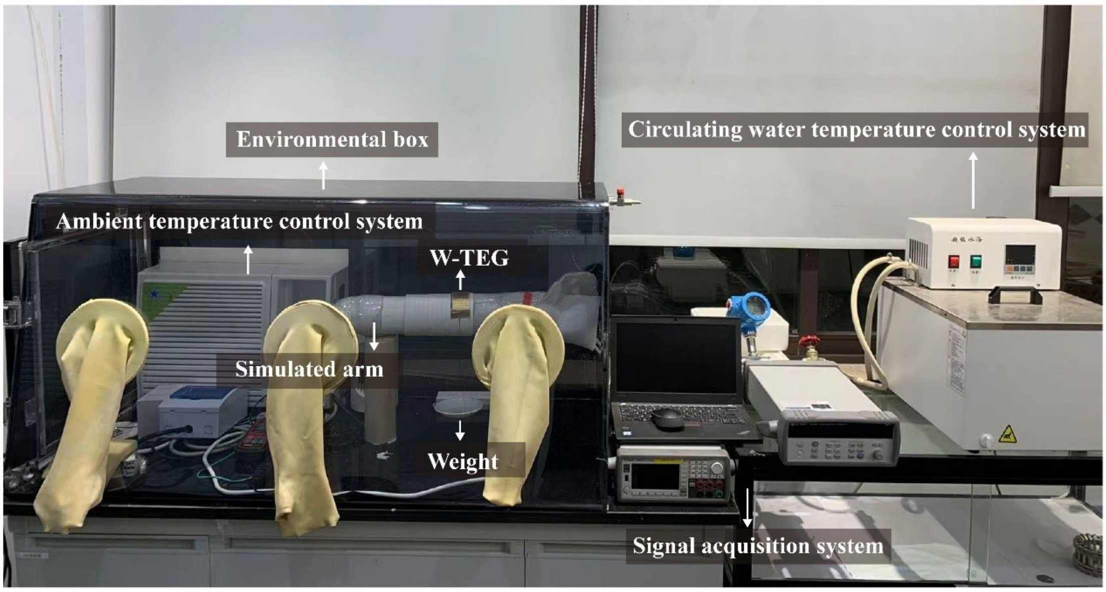


Figure S9. Simulation arm test system for W-TEG power generation performance characterization.

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