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RESEARCH ARTICLE

# Nanophononic metamaterials induced proximity effect in heat flux regulation

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## Supporting Information

In this work, the Nose–Hoover thermostat is chosen to control the temperature, which updates not only the velocity but also the position of the atoms, as follows [1]:

$$\frac{d}{dt}p_i = F_i - \eta p_i, \tag{S.1}$$

$$\frac{d}{dt}\eta = \frac{1}{\tau^2}\left[\frac{T(t)}{T_0} - 1\right], \tag{S.2}$$

$$T(t) = \frac{2}{3Nk_B}\sum_i \frac{p_i^2}{2m_i}, \tag{S.3}$$

where $i$ is the atomic label, $p$ is momentum, $m$ is the mass, and $F$ is the force. $\eta$ and $\tau$ are the dynamic parameters and relaxation times, $k_B$ is the Boltzmann constant, and $N$ is the number of atoms.

Here the temperature is calculated by this definition,

$$\sum_i \varepsilon_i = \frac{dim}{2}k_B NT, \tag{S.4}$$

where $i$ is the atomic label, $\varepsilon$ is the kinetic energy, in our system $dim=3$. Heat flux can be calculated by the following equation,

$$\mathbf{J} = \frac{1}{V}\left[\sum_i e_i \mathbf{v}_i - \sum_i \mathbf{S}_i \mathbf{v}_i\right], \tag{S.5}$$

where **J** is the heat flux, $V$ is the volume, $i$ is the atomic label, $e$ is the energy, **S** is the stress tensor, and $v$ is the velocity vector. Heat flux in different directions can be calculated using the following equation,

$$J_x = \frac{1}{V}\left[\sum_i e_i v_{xi} - \sum_i \left(S_{ixx}v_{ix} + S_{ixy}v_{iy} + S_{ixz}v_{iz}\right)\right], \tag{S.6}$$

$$J_y = \frac{1}{V}\left[\sum_i e_i v_{yi} - \sum_i \left(S_{iyx}v_{ix} + S_{iyy}v_{iy} + S_{iyz}v_{iz}\right)\right], \tag{S.7}$$

$$J_z = \frac{1}{V}\left[\sum_i e_i v_{zi} - \sum_i \left(S_{izx}v_{ix} + S_{izy}v_{iy} + S_{izz}v_{iz}\right)\right], \tag{S.8}$$

We calculate the location-dependent heat flux distribution along the y-axis, in arrays P1–P7. Fig. S1 and Fig. S2 show the heat flux spatial distribution of the regulator in the pristine silicon film and nanopillar height of 25 UC, respectively. For the pristine silicon film, the heat flux from P1 to P7 shows a uniform distribution, while for the regulator, in regions of P5–P7, the local heat flux along the *y*-axis is spatially homogeneously distributed. On the other side, in regions P2&P3, the local heat flux in the functional region is obviously lower than that in the pristine section. However, in regions P1 & P4, particularly in P1, compared with the pristine section, there is a dramatic reduction in local heat flux in the central part, although no nanopillars are there. Clearly, the nanopillars induce non-localization modulation in heat flux or the heat flux proximity effect. The heat flux at the center is 0.78 of that at the edges, indicating that the heat flux regulation is achieved due to the presence of the nanopillar around the studied section.

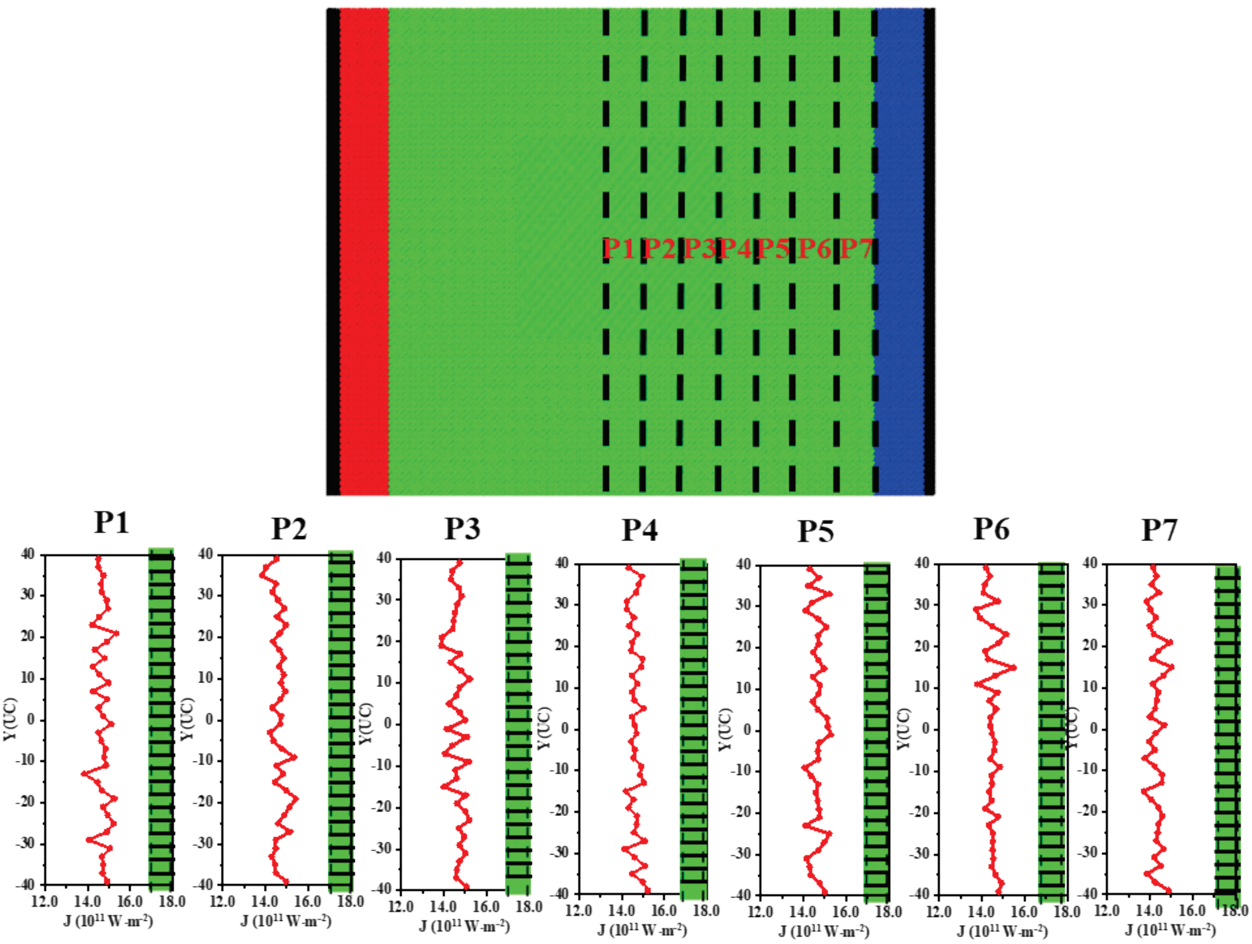


**Fig. S1** The heat flux spatial distribution of the pristine film.

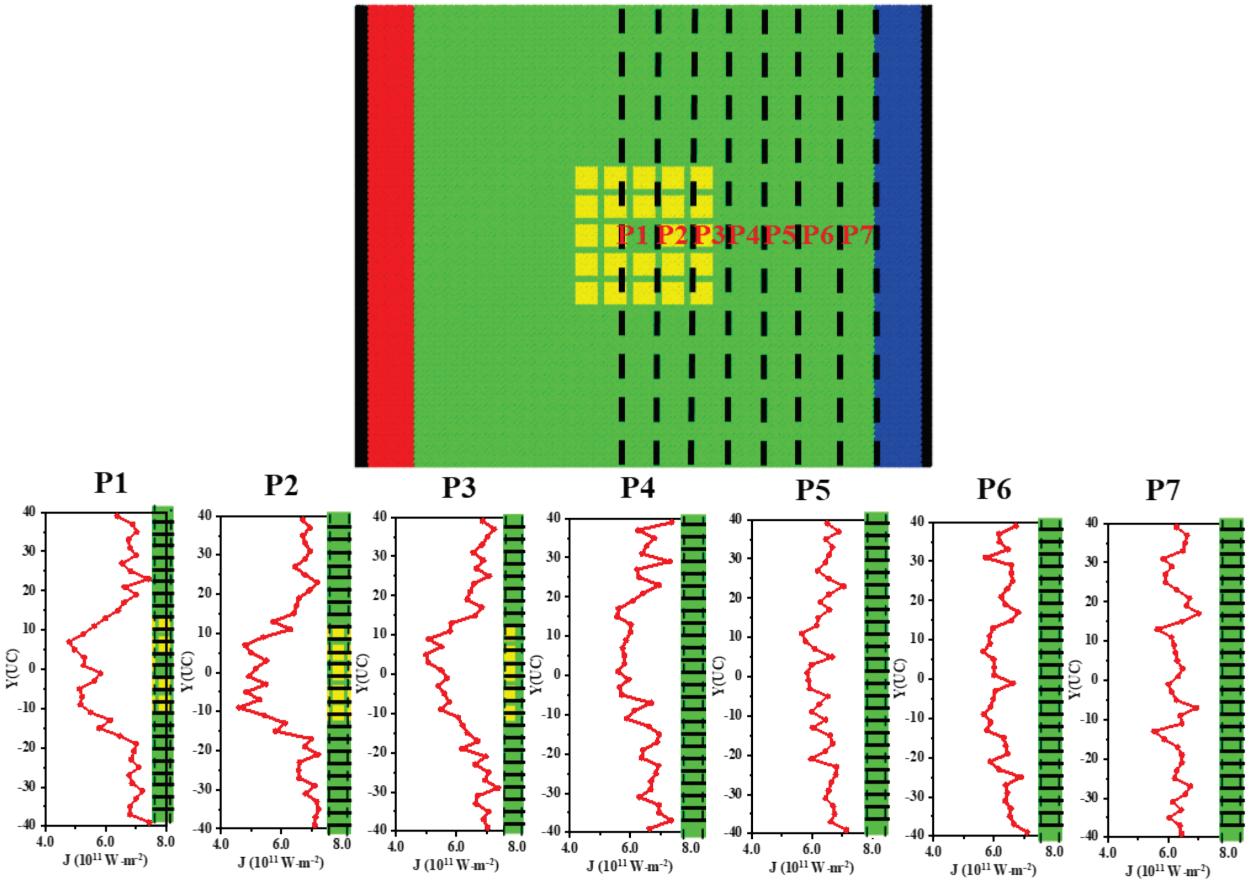


**Fig. S2** The heat flux spatial distribution in region P1–P7 of the regulator with the nanopillar height of 25 UC.

Fig. S3 shows the intensity of localized phonon modes in the regulator with the nanopillar height of 25 UC. It is clear that the localized modes are distributed in the functional region, and it is low in the pristine region and even in the center of the functional region. These results provide a direct demonstration that localization takes place within the functional regions. Although there is no obvious localization mode in the central region, its local heat flux is significantly reduced due to the proximity effect induced by the nanopillar region.

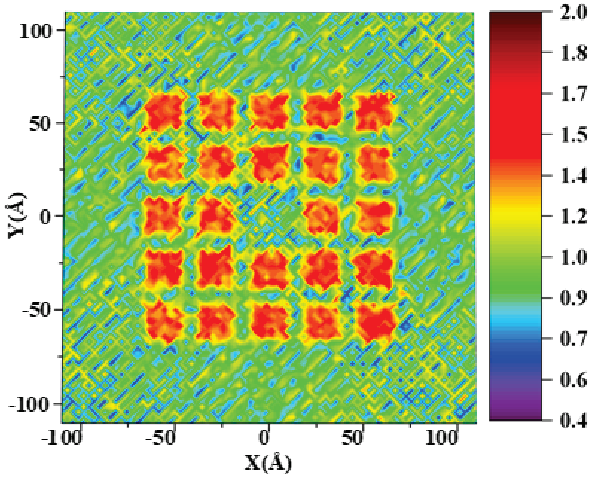


**Fig. S3** The intensity of localized phonon modes in regulator with the nanopillar height of 25 UC.

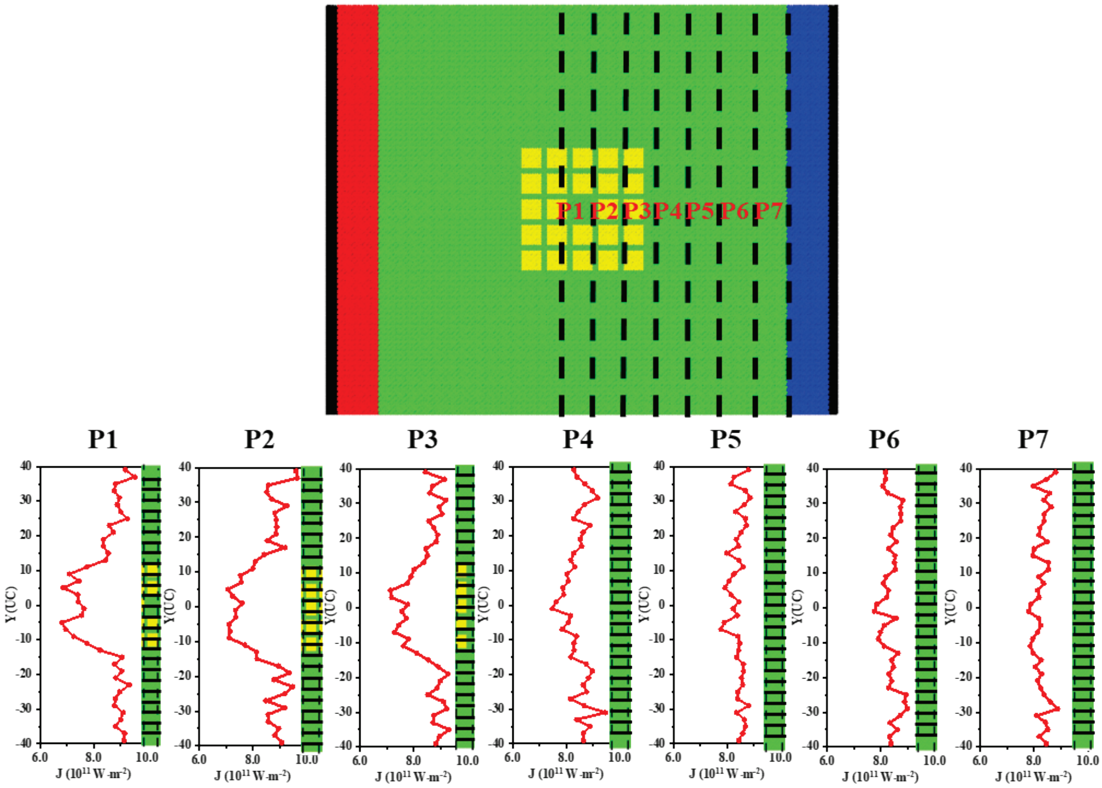


**Fig. S4** The heat flux spatial distribution of the regulator in region P1–P7 with the host nanofilm thickness is 10 UC.

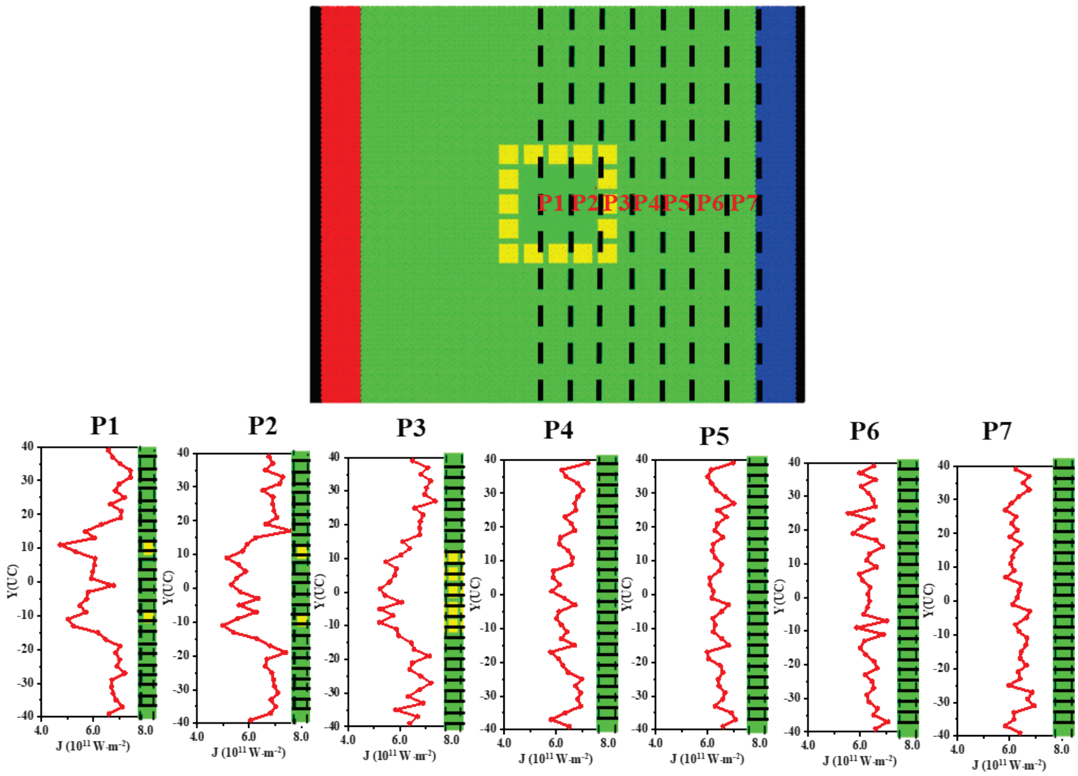


**Fig. S5** The heat flux spatial distribution in region P1–P7 of the regulator with the number of nanopillar rows is 1.

**References**

1. H. J. C. Berendsen, J. P. M. Postma, W. F. V. Gunsteren, A. DiNola, and J. R. Haak, Molecular dynamics with coupling to an external bath, *J. Chem. Phys.* 81, 3684 (1984) https://doi.org/10.1063/1.448118