Supplemental material for:
Phonon Lateral Confinement Enables Thermal Rectification in Asymmetric Single-Material Nanostructures

Yan Wang,[1,2] Ajit Vallabhaneni,[1,2] Jiuning Hu,[2,3]
Bo Qiu,[1,2] Yong P. Chen,[2,3,4] and Xiulin Ruan[1,2,*]

[1]*School of Mechanical Engineering, Purdue University, West Lafayette, Indiana 47907, USA*

[2]*Birck Nanotechnology Center,Purdue University, West Lafayette, Indiana 47907, USA*

[3]*School of Electrical and Computer Engineering, Purdue University, West Lafayette, Indiana 47907, USA*

[4]*Department of Physics, Purdue University, West Lafayette, Indiana 47907, USA*

(Dated: December 16, 2013)

I. DETAILED PROOF OF THE ABSENCE OF THERMAL RECTIFICATION IN BULK SINGLE MATERIAL

For the insulated (adiabatic) surfaces S_{ins}'s shown in Fig. 2, we have $\frac{\partial T}{\partial \vec{\nu}}|_{S_{ins}} = 0$, where $\vec{\nu}$ is the surface normal vector. Heat conduction is governed by the heat diffusion equation,

$$\vec{\nabla} \cdot \left\{ \kappa \left[T \left(\vec{x} \right) \right] \cdot \vec{\nabla} T \left(\vec{x} \right) \right\} = 0, \tag{S1}$$

where κ is the thermal conductivity tensor which only depends on temperature in the bulk regime, but it is not necessarily isotropic. If we set the axes of the coordinate system along the principal directions, i.e., κ is diagonal, we can linearize Eq. S1 through the Kirchhoff transformation by defining a new quantity, $K_i(T) = \int_\epsilon^T \kappa_{i,i}(T)dT + \kappa_{i,i}(\epsilon)$, where κ_{ii} is the ith component of the diagonal of the thermal conductivity tensor. It is evident that $\kappa_{i,i}(T) = \frac{\partial K_i(T)}{\partial T}$. Physically, ϵ can be of any non-negative value as long as it is lower than any phase-change temperature. Therefore,

$$\kappa_{i,i}[T(\vec{x})] \cdot \frac{\partial T(\vec{x})}{\partial x_i} = \frac{\partial K_i[T(\vec{x})]}{\partial x_i}, \tag{S2}$$

and Eq. S1 becomes

$$\sum_i \frac{\partial^2 K_i}{\partial x_i^2} = 0. \tag{S3}$$

For the $forward$ and *backward* cases, the only difference regarding Eq. S3 is the boundary conditions at the two surfaces S_1 and S_2. We now have a complete set of partial differential equations together with boundary conditions for the two cases, which are

$$\begin{cases} \sum_{i=1}^{N} \frac{\partial^2 K_{i,f}}{\partial x_i^2} = 0, \\ \frac{\partial K_f}{\partial \vec{\nu}}|_{S_{ins}} = 0, \\ K_{i,f}|_{S_1} = K_i(T_{hot}), \\ K_{i,f}|_{S_2} = K_i(T_{cold}), \end{cases} \tag{S4}$$

for the *forward* case, and

$$\begin{cases} \sum_{i=1}^{N} \frac{\partial^2 K_{i,b}}{\partial x_i^2} = 0, \\ \frac{\partial K_b}{\partial \vec{\nu}}|_{S_{ins}} = 0, \\ K_{i,b}|_{S_1} = K_i(T_{cold}), \\ K_{i,b}|_{S_2} = K_i(T_{hot}), \end{cases} \tag{S5}$$

for the *backward* case, respectively. Summing up Eqs. S4 and S5 generates

$$\begin{cases} \sum_{i=1}^{N} \frac{\partial^2 K_{i,t}}{\partial x_i^2} = 0 \\ \frac{\partial K_t}{\partial \vec{\nu}}|_{S_{ins}} = 0, \\ K_{i,t}|_{S_1} = K_i(T_{hot}) + K_i(T_{cold}), \\ K_{i,t}|_{S_2} = K_i(T_{cold}) + K_i(T_{hot}). \end{cases} \tag{S6}$$

where we have defined $K_{i,t}[T(\vec{x})] = K_{i,f}[T(\vec{x})] + K_{i,b}[T(\vec{x})]$. The subscripts f, b, and t stand for "forward", "backward", and "total", respectively.

The solution to Eq. S6 is unique and must be a constant

$$K_{i,t} = K_i(T_{hot}) + K_i(T_{cold}) = const. \tag{S7}$$

Therefore,

$$\frac{\partial K_{i,t}}{\partial x_i} = \frac{\partial K_{i,f}}{\partial x_i} + \frac{\partial K_{i,b}}{\partial x_i} = 0. \tag{S8}$$

Plugging in Eq. S2 leads to Eq. 2 in the main text.

II. NUMERICAL VERIFICATION OF THE ABSENCE OF THERMAL RECTIFICATION IN BULK SINGLE MATERIAL

To verify the analytical proof of the absence of thermal rectification in asymmetric bulk single material, we use the finite element method with Ansys to solve a 2D heat transfer problem. The structure is a right trapzoid, as shown in the inset of Fig. S1. For the *forward* case, the temperature is maintained at 600 K on the left end, and 10 K on the right end, and vice versa for *backward.* We consider both isotropic κ and anisotropic κ cases, and the results are plotted in Fig. S1 and Fig. S2, respectively, with the κ-T curves in Fig. S3.

We select an arbitrary path across the structure, and measure the the heat flux vector $\vec{J}''$ as a function of position on this path. In both Fig. S1 and Fig. S2, the heat flux vectors at any position are same in magnitude but opposite in direction for *forward* and *backward* cases. The results verifies our analytical proof of the absence of thermal rectification in asymmetric bulk-size single material.

* Electronic address: ruan@purdue.edu

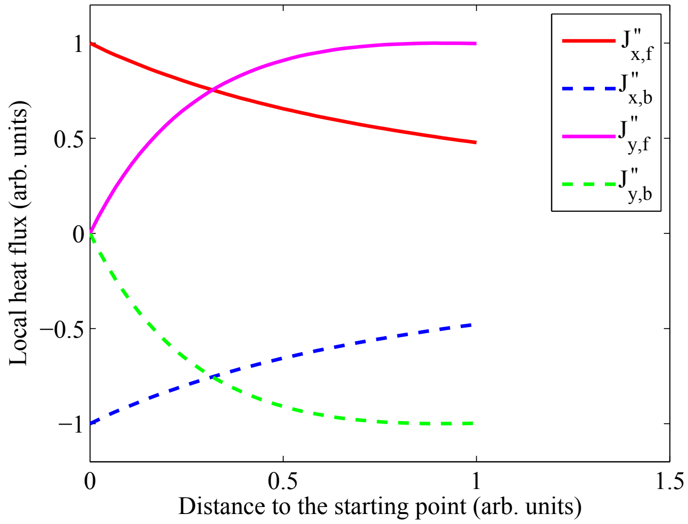

FIG. S2: Numerical verification for anisotropic κ, i.e., $\kappa_{xx} \neq \kappa_{yy}$.

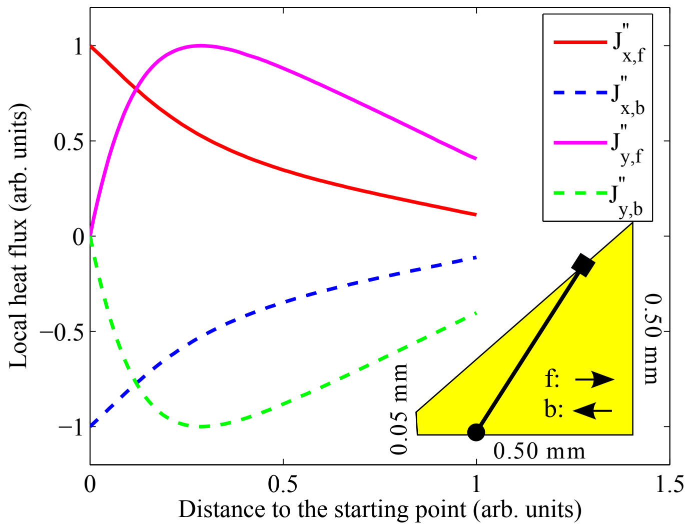

FIG. S1: Numerical verification for isotropic κ. The inset is the structure used for the numerical calculations. The heat flux, which has x and the y components, is measured along an arbitrary path (from the filled circle to the filled square) as a function of the distance to the starting point. f and b represent *forward* and *backward* cases, respectively.

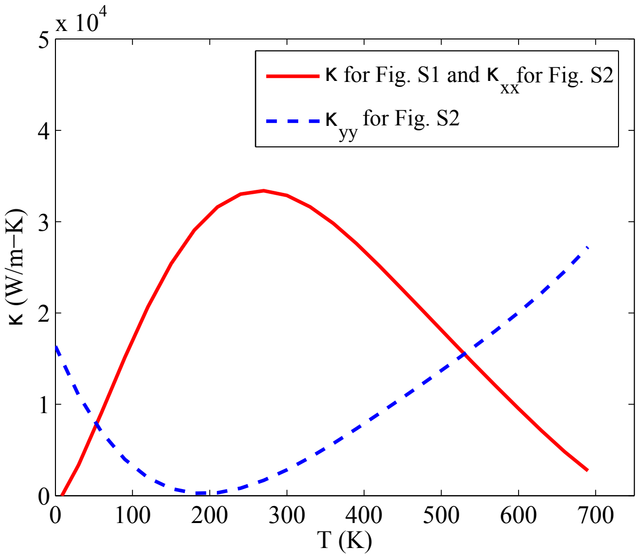

FIG. S3: κ's used for the isotropic case in Fig. S1 and the anisotropic case in Fig. S2.