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Thermal diode using controlled capillary in heterogeneous nanopores

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ABSTRACT

The development of a compact, efficient, reliable thermal diode is crucial to improve advanced thermal management efficiency and controllability, and to enable brand new applications such as thermal logic gates and computers. In this study, we examine a nanoscale and efficient capillary-controlled thermal diode mechanism in Ar-filled Pt-based heterogeneous nanoporous structures, using Grand Canonical Monte Carlo (GCMC) simulation combined with Non-Equilibrium Molecular Dynamics (NEMD) simulation at the temperature range of 70–150 K and the pressure of 1.66 atm. Results show that the large thermal conductivity contrast between the controlled adsorption and capillary states using the structural heterogeneity (nanopillars on only one surface) and/or material heterogeneity (two different materials for nanogap surfaces) allows for the maximum thermal rectification ratio, $R_{max} \sim 140$ with minimal hysteresis under the cyclic operating temperatures $-40\text{ K} < \Delta T < +40\text{ K}$. It is also found that the material heterogeneity is equivalent to the structural heterogeneity for minimizing the hysteresis in adsorption-capillary transition, but the heat flux across the nanogap with the material heterogeneity reduces due to weaker Ar-solid interaction. The coupled structural-material heterogeneity for the capillary-driven thermal diode is also discussed. The obtained results pave pathways for advanced thermal management systems such as thermal transistors, thermal logic gates, and computers.

1. Introduction

A thermal diode is a key component to substantially improve the operating energy efficiency in waste heat recovery [1–3], smart building [4] systems, and even open brand new applications including thermal logic gates and computers [5–9]. The thermal diode (rectifier) allows for an asymmetric heat flux, i.e., favorable heat flux in only one direction of the temperature gradient. The thermal diodicity (or rectification) ratio, *R*, is defined as

$$R = \frac{|\boldsymbol{q}_+| - |\boldsymbol{q}_-|}{|\boldsymbol{q}_-|}, \tag{1}$$

where $|\boldsymbol{q}_+|$ and $|\boldsymbol{q}_-|$ are the heat fluxes in the positive (favorable) and negative (unfavorable) directions, respectively, and the thermal diode requires $R > 0$.

Various diode designs have employed nonlinear heat transfer characteristics, both experimentally and theoretically, and detailed literature review is available in recent studies [8,10,11]. Thermal diode has been predominantly explored in nonlinear thermal conduction mechanisms, as the first thermal diode mechanism has been demonstrated by the asymmetric thermal conductivity through Cu/CuO interface [12]. The nonlinear conduction-based thermal diodes have employed the asymmetric phononic thermal transport through heterogeneous solid-solid junctions [3,13–20], heterogeneous solid-liquid junctions [21–23], heterogeneity in asymmetric geometries [6,7,18,24–46], or heterogeneity with asymmetric mass distribution [32,47–49] without the external energy control. The thermal diode has also been explored with the assistance of the external energy controllers [50–56]. Asymmetric free electron thermal transport across heterogeneous interfaces has been also explored and thermal diodicity is demonstrated due to tailored electron transport through conducting/insulating materials (macroscale) or in quantum state (atomic-scale) [57–59]. Other conduction-based designs include electrochemically tuned thermal conductivity change during delithiation of $LiCoO_2$ [60], shape memory alloy-based passive solid state diode [61], and liquid-state thermal expansion-based thermal diode [62]. Thermal rectification has been also achieved through the asymmetric liquid-solid or gas-solid thermal conductivity near the rough surface [63].

The thermal diode has been also achieved by capillary-assisted nonlinear heat transfer in heat pipes [64,65], heterogeneous water wetting using hydrophobic and hydrophilic surfaces [66,67], or gravity-driven asymmetric natural convection between solid plates [10,68]. Here, the primary working principle is to utilize

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Nomenclature

F	interactive force, N
FCC	Face Centered Cubic
GCMC	Grand Canonical Monte Carlo
L	nanogap size, m
l	nanopillar height, m
m	mass, kg
NEMD	Non-Equilibrium Molecular Dynamics
NVT	canonical ensemble
p	pressure, Pa
q	heat flux, W/m^2
r	interatomic distance, m
R	thermal rectification ratio
T	temperature, K
TAC	thermal accommodation coefficient
u	velocity, m/s
V	volume, m^3

Greek symbols

Γ	spring potential constant, N/m
ε	Lennard-Jones energy constant, J
σ	Lennard-Jones zero potential distance, m
φ	interatomic potential, J

Subscripts

ff	fluid-fluid
g	gas
sf	solid-fluid
tr	capillary transition
x	x-direction
y	y-direction
z	z-direction
+	positive heat flux direction
–	negative heat flux direction

the asymmetric thermofluid transport, which in turn allows for the efficient thermal diodicity. However, those have been demonstrated at macro-scale systems.

The nonlinear radiation-based thermal diode has utilized photon transport in tailored micro/nanostructures using temperature-dependent optical resonance [69,70], dielectric coating [71], different doping concentration [72,73], phase-change radiation [74,75], blackbody sandwiched by plates with different emissivity [10,76], or by near-field nano-thermomechanical rectification [77].

Several studies have demonstrated the thermal diode effect in quantum (atomic-scale) systems such as heterogeneous junctions [78], nonlinear electron-gas-dispersion relation transport [79,80], quantum dot structure [2,81,82], or nonlinear quantum circuits [83]. Despite interesting scientific phenomena and approaches, the thermal diode effect in quantum systems primarily remains in theoretical approaches.

Although various theoretical approaches have been explored for the thermal diode, thermal rectification ratio in the experiments remains poor, especially at nano-/microscale [6,9,12,28,60,77], primarily due to challenging manufacturing and expensive operations [6,10,84–86]. Indeed, efficient thermal diodes have been experimentally demonstrated in nonlinear convection mechanisms [10,64–68,87,88], but they require bulky systems, which limits the system mobility and leads to slow transient response. Also, the radiation-based thermal diodes require very high operating temperatures, which may limit the practical applications.

To overcome aforementioned challenges, a new class of thermal diode is examined by employing the large thermal conductivity contrast between gas (adsorption) and liquid (capillary) states in heterogeneous nanoporous structures, so called capillary-controlled thermal diode. The effects of the structural/material heterogeneity on the thermal diode have been explored using Ar-filled Pt-based nanogap and Grand Canonical Monte Carlo (GCMC) simulation combined with Non-Equilibrium Molecular Dynamics (NEMD) simulation. It is noteworthy that the working principle of the diode in present study is fundamentally different from the previous study by the authors, so called adsorption-controlled thermal diode [89,90]. The previous work employs the adsorption-controlled interfacial heat transfer via Thermal Accommodation Coefficient (TAC) coupled with adsorption-controlled gas pressure changes inside the heterogeneous nanogap (material heterogeneity only), while the present study utilizes the large thermal conductivity contrast between the gas and capillary states via the adsorption-capillary morphological transition controlled by structural and/or material heterogeneity. Also, the previous work has no structural heterogeneity, i.e., nanogap with two different materials without nanopillars, while the present study uses the structural heterogeneity (nanogap with nanopillars on only one surface) for a controlled adsorption-capillary transition with a minimal hysteresis.

2. Working principle

The key working principle of the capillary-controlled-based thermal diode is to employ the large contrast in thermal conductivity between the gas (adsorption) and liquid (capillary) states in nanopores. In fact, the capillary transition inherently brings hysteresis for the capillary condensation/evaporation under the cyclic operations [91,92], which in turn results in poor controllability in the thermal diode operation. To improve the operational controllability, the structural heterogeneity, i.e., nanopillars on one surface only is employed as shown in Fig. 1. Ar particles fill the nanogap with the size L_z as thermal energy carriers between the surfaces, and morphological Ar state, i.e., adsorption or capillary, regulates the heat flux magnitude, mainly due to Ar number density. The

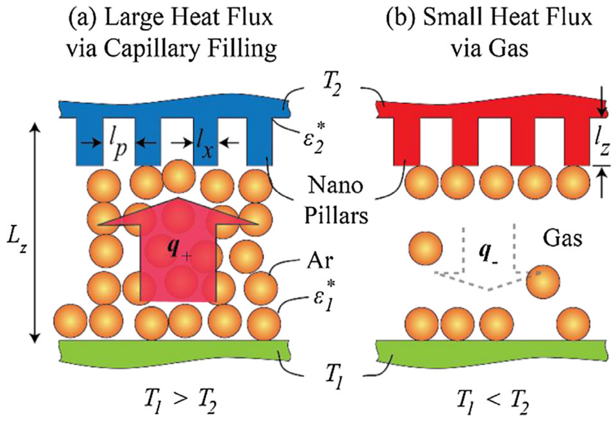

Fig. 1. Schematic of capillary-controlled thermal diode using Ar-filled Pt-based heterogeneous nanogap (a) $q_+ \gg 0$ for $T_1 > T_2$ due to the high thermal conductivity of liquid-like (capillary) state, and (b) $q_- \sim 0$ for $T_1 < T_2$ due to the low thermal conductivity of gas (adsorption) state. The surface temperatures, T_1 and T_2, heat fluxes, q_+, and q_-, dimensionless fluid-solid interactions, ε_1^* and ε_2^*, nanogap and nanopillar size parameters, L_z, l_p, l_x, l_z, and Ar particles are also shown.