Applied Energy xxx (xxxx) xxx–xxx

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

# A detailed study on phonon transport in thin silicon membranes with phononic crystal nanostructures

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## HIGHLIGHTS

- Influences of period length and porosity on different phonon branches are investigated.
- Effects of pore configuration and placement on phonon transports are checked.
- The major geometric parameter, which affects phonon transport greatly, is determined.
- A nonlinear regression model is obtained for predicting the thermal conductivity.

## ARTICLE INFO

*Keywords:*
Phonon transport
Phononic crystal nanostructures
Lattice thermal conductivity
Boltzmann transport equation
Discrete ordinates method

## ABSTRACT

A common method to improve thermoelectric performance is to reduce thermal conductivity by enhancing phonon scattering. In this paper, a frequency-dependent phonon radiative transport equation (PRTE) solver, based on the discrete ordinates method, is developed to simulate phonon transport in thin silicon membranes with phononic crystal nanostructures. The influence of geometric parameters on phonon transport is discussed in detail. Besides, a nonlinear regression model is attained for predicting the thermal conductivity of thin silicon membranes with phononic crystal nanostructures using the non-linear least-squares method. The results indicate that thermal conductivity is reduced by phononic crystal nanostructures mainly due to the back scattering of phonons with pore boundaries, and phonons with larger mean free path have stronger back scattering. When the pore placement is fixed, pore configuration affects phonon transport in thin silicon membranes with phononic crystal nanostructures. In addition, thermal conductivity is primarily controlled by three geometric parameters, including $r_{\perp}$, $r_{||}$, and $A_u$. Moreover, the obtained regression model reveals the relationship between thermal conductivity and geometric parameters well, which can offer useful suggestions for fabricating thin silicon membranes with low thermal conductivity.

## 1. Introduction

Rapidly increased energy consumption and serious environmental problems have been one of the most important global issues, which have enormous influence on the suitable development of economic and society. To ensure energy security and also meet climate mitigation goals, efficient utilization of renewable energy, such as wind energy and solar energy, has aroused great interests [1–4]. Photovoltaic (PV) and concentrating solar power (CSP) are two main types of solar energy technologies. CSP technologies, mainly including parabolic trough collector [5–8], parabolic dish collector [9–11], linear Fresnel reflector [12–14], solar power tower [15–18], etc., are used primarily in large power plants. Comparing with CSP system, PV system is more flexible and inexpensive, which can be built to meet different electric power need. As a promising technology, photovoltaic cells have been rapidly developed over past decades [19–22]. When the sun light strikes photovoltaic cells, electron-hole pairs are activated by photons with energy greater than the band-gap energy, while photons with energy lower than the band-gap energy are absorbed and transformed into heat resulting in temperature increase of photovoltaic cells. The increased temperature would decrease the efficiency of photovoltaic cells. To overcome this drawback and enhance the utilization of solar energy, a PV-TE (photovoltaic-thermoelectric) hybrid system has been proposed [23–28]. By converting exhaust heat generated in the photovoltaic cells to electricity through the thermoelectric module, researches show that efficiency of the hybrid system is significantly increased compared with

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http://dx.doi.org/10.1016/j.apenergy.2017.07.083
Received 19 January 2017; Received in revised form 21 July 2017; Accepted 22 July 2017

**Nomenclature**

| | |
|---|---|
| $a$ | lattice constant (Å) |
| $A_p$ | area of a pore ($nm^2$) |
| $A_u$ | area of a unit cell ($nm^2$) |
| $b$ | pore length (nm) |
| D | density of states ($s\,rad^{-1}\,m^3$) |
| $f$ | distribution function of phonons |
| $I$ | directional phonon intensity ($J\,m^{-2}\,sr^{-1}$) |
| $k_B$ | Boltzmann constant ($J\,K^{-1}$) |
| $L$ | period length (nm) |
| $\langle n \rangle$ | Bose-Einstein distribution |
| $p_B$ | boundary specularity |
| $p$ | phonon branch |
| $\bar{q}$ | average heat flux ($W\,m^{-2}$) |
| $\boldsymbol{q}$ | wave vector ($m^{-1}$) |
| $\boldsymbol{r}$ | position vector for phonons (nm) |
| $r$ | ratio between lengths |
| $S$ | Seebeck coefficient ($V\,K^{-1}$) |
| $\hat{\boldsymbol{s}}$ | unit vector of phonon transport direction |
| $t$ | time (s) |
| $T$ | temperature (K) |
| $\boldsymbol{v}$ | velocity vector ($m\,s^{-1}$) |
| $\boldsymbol{v}_g$ | phonon group velocity ($m\,s^{-1}$) |
| $w_k$ | quadrature weights associated with the direction $\hat{\boldsymbol{s}}_k$ |
| $Z$ | figure of merit ($K^{-1}$) |
| $ZT$ | dimensionless figure of merit |

*Greek symbols*

| | |
|---|---|
| $\hbar$ | Reduced Planck constant (J s) |
| $\sigma$ | electrical conductivity ($\Omega^{-1}\,m^{-1}$) |
| $\lambda$ | thermal conductivity ($W\,m^{-1}\,K^{-1}$) |
| $\varphi$ | porosity |
| $\tau$ | relaxation time (s) |
| $\xi$, $\eta$, $\mu$ | elements of unit vector |
| $\theta$ | polar angle (rad) |
| $\psi$ | azimuthal angle (rad) |
| $\omega$ | angular frequency ($rad\,s^{-1}$) |

*subscript*

| | |
|---|---|
| 0 | equilibrium |
| Left | left side of the unit cell |
| N | normal process of three phonon scattering |
| NU | normal process and Umklapp process of three phonon scattering |
| p | pore |
| Right | right side of the unit cell |
| u | unit cell |
| U | Umklapp process of three phonon scattering |
| $\perp$ | direction perpendicular to heat flux |
| $\parallel$ | direction parallel to heat flux |

that of photovoltaic cells [25,26]. The optimum thermoelectric materials could help the efficiency increase up to 50% [23].

The ideal thermoelectric property of materials is evaluated by the dimensionless thermoelectric figure of merit ($ZT$), which is defined as $ZT = (\sigma S^2/\lambda)T$, where $\sigma$ is the electrical conductivity, $S$ is the seebeck coefficient, $\lambda$ is the thermal conductivity, and $T$ is the absolute temperature [29]. For the utilization in the PV-TE hybrid system, thermoelectric modules with high $ZT$ at room temperature are preferred due to the temperature limit of photovoltaic cells. At present, $Bi_2Te_3$ is the most commonly used thermoelectric material, which has the dimensionless figure of merit $ZT$ above 1.0 at room temperature. Unfortunately, its application is confined by low stability and high manufacturing cost. On the other hand, silicon has attracted more and more attention because of its abundance and mature processing technology. However, due to the high thermal conductivity ($149\,W\,m^{-1}\,K^{-1}$ at room temperature) of silicon, its dimensionless figure of merit is small. Many efforts have been devoted to increase its dimensionless figure of merit by reducing the thermal conductivity. Enhancing phonon scattering by introducing nanostructures has been proved to be an effective approach to reduce the thermal conductivity because heat is mainly transported by phonons in silicon. Accordingly, several phononic crystals (PnCs) with enhanced $ZT$ have been fabricated and tested. By introducing nanostructures in p-type SiGe alloys, Chen et al. [30] reported a remarkable improvement on the peak $ZT$ from 0.65 to 0.95 at 1073–1173 K. Furthermore, a $ZT$ of 1.2 in p-type nanostructured SiGe alloys at 1173 K was achieved by creating defects during nanostructuring [31]. Furthermore, Chen et al. [32] fabricated nanostructured bulk silicon by high-energy ball milling and hot pressing. Their experimental data shows that nanostructured bulk Si samples exhibit very large reduction in thermal conductivity with values around $10\,W\,m^{-1}\,K^{-1}$. And an exceptional increase in the $ZT$ of bulk Si by a factor of nearly 3.5 is observed. Using high-pressure torsion (HPT), Harish et al. [33] obtained the HPT-processed samples of bulk crystal silicon. The lattice thermal conductivity of these samples, measured by picosecond time domain thermoreflectance, is approximately $7.6\,W\,m^{-1}\,K^{-1}$, which is nearly one-twentieth of the intrinsic single crystalline value. The thermal conductivity can be further reduced for silicon membranes due to the phonon size effect in thin film. Yang et al. [34] fabricated thin silicon membranes with nanoscopic holes, which are called phononic crystal nanostructures, by nanosphere lithography or block copolymer lithography. The measured lowest thermal conductivity for intrinsic samples is about $2.03\,W\,m^{-1}\,K^{-1}$. And the $ZT$ of these fabricated samples is dramatically increased from 0.01 for the bulk to 0.4 at the room temperature. It was demonstrated that the thermal conductivity of thin silicon membranes with phononic crystal nanostructures can be even smaller than that of an array of nanowires, and their electrical conductivity is bulk-like [35]. Using time domain thermoreflectance, Hopkin et al. [36] measured the thermal conductivity of a series of single crystalline silicon PnCs. The measured thermal conductivity is much lower than the predicted values considering boundary scattering only, which indicates that not only boundary scattering but also coherent phononic effects result in the reduction of the cross plane thermal conductivity. In addition, Nomura et al. [37] compared phonon transport in Si phononic crystal nanostructures with square-lattice and triangular-lattice. They found that triangular-lattice Si phononic crystal nanostructures have lower thermal conductivity compared with square-lattice, and the largest difference was about 20% when the porosity was around 30%. Wagner et al. [38] analyzed the influence of disorder on phononic properties of 2D phononic crystals by femtosecond time-domain spectroscopy and finite element method simulations. It was found that the disorder in PnCs has enormous impact on hypersonic phonon spectrum, which would result in the suppression of coherent acoustic phonon modes. To gain an insight into the phonon transport in PnCs and fabricate PnCs with lower thermal conductivity, several numerical methods have been developed, including density-functional perturbation theory (DFPT) [39,40], Molecular Dynamics (MD) [41,42], and Phonon Boltzmann transport equation [43–45].

In the previous works, the effects of disorder and porosity on phonon transport in the thin silicon membranes with phononic crystal nanostructure have been studied. But the influence of phononic crystal nanostructures on different phonon branches is still indistinct. And little