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Thermoelectric Conversion Performance of Porous Si Thin Film — Phonon Transport Simulation —

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Abstract – Porous semiconductor materials can effectively scatter phonons, often showing good performance of thermoelectric conversion, depending on their spatial scale of structure. In this study, phonon transport in several types of porous silicon thin films was numerically investigated based on the Boltzmann transport equation combined with the relaxation time approximation to evaluate the thermal conductivity. The films were modelled as an assembly of particles with given size, which resembles sintered Si films. Structural analysis indicates that the porosity determines the electric conductivity while phonon transport is more suppressed in films of smaller particles, suggesting that film structures can be optimized by controlling the pore size.

***Keywords*:** Thermoelectric conversion; Figure of merit; Phonon transport; Porous film; Tortuosity; Numerical simulation; Boltzmann transport equation; Extended VOF scheme

1. Introduction

Thermoelectric energy conversions by utilizing the Seebeck effect have attracted much attention recently [1]. To improve the conversion efficiency, control of phonon propagation with nano-scale structures is very popular [2], which is based on the difference of mean free path (MFP) between phonons and electric charge carriers (electrons and holes). In typical cases with silicon-base devices, MFP of phonons is in an order of 100–1000 nm while that of electrons is 1–10 nm. Thus, structures of 10–100 nm size are expected to be effective for suppressing the phonon heat transfer, leading to better conversion efficiency.

In this study, we focus on porous films fabricated by sintering semiconductor fine powders [3]; control of experimental conditions seems to give nano-scale structures in a range suitable for phonon transport suppression. To investigate the transport properties of such porous films, we construct a two-dimensional model based on randomly arranged particles and simulate the phonon transport through the modelled film. Combined with the electric conductivity analysis, the improvement of thermoelectric conversion efficiency is evaluated.

2. Methods

We develop a variety of nano-porous silicon film models and investigate the transport properties to evaluate the thermoelectric performance. All simulations were done for two-dimensional systems (i.e., thin film) to save the computational resources.

2.1. Phonon Transport

We have developed an extended VOF scheme to simulate the phonon transport in micro scales [4, 5], which solves the Boltzmann transport equation (BTE) for the phonon distribution function $f(\vec{k};\vec{r},t)$ in the reciprocal space of wave number $\vec{k}$ at position $\vec{r}$ and time t with the relaxation time approximation [1], as

$$\frac{\partial f}{\partial t}+\vec{v}\frac{\partial f}{\partial \vec{r}}=-\frac{f-f^{eq}}{\tau(\omega)} \tag{1}$$

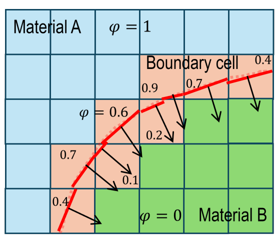
where $f^{eq}(T)$ is the equilibrium distribution function at temperature T. The phonon group velocity $\vec{v}$ is evaluated from a dispersion relation of the angular frequency $\omega(\vec{k})$. For simplicity we here consider a single acoustic branch in an isotropic medium [4] as

$$\omega(\vec{k}) = \omega_{\max}\left|\sin\frac{1}{2}ka\right| \tag{2}$$

where a is the lattice constant. Also a simple form is assumed as the relaxation time

$$\tau = \frac{\tau_0}{0.1 + |k/k_{\max}|^2} \tag{3}$$

With an appropriate choice of parameters (a, $\omega_{\max}$, $k_{\max}$, and τ_0), we can simulate the phonon transport in silicon crystals; see Ref. [4] for details. The cumulative thermal conductivity of our model gives 50 % at the mean free path ~ 350 nm, similar to more realistic Si models. To numerically solve Eq. (1) with appropriate boundary conditions (typically contacting two heat baths of different temperatures along the x direction while periodic along the y direction) and initial conditions, we adopt a finite difference method, combined with an extended VOF (volume of fluid) scheme to treat the structure surface (phonon reflection and transmission at the surface) as schematically shown in Figure 1. The ratio of specular reflection α is a parameter for the boundary, and $\alpha = 0.5$ is chosen in this study.



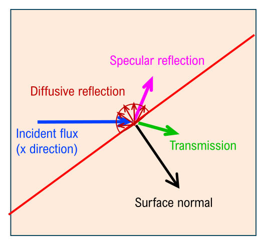


Fig. 1: Schematic view of the developed extended VOF method [4], indicating (left) boundary cells with surface normal, and (right) treatment of phonon transport at the boundary. The VOF value φ is assigned to each simulation cell, which represents the ratio of "Material A", thus the cell with $0 < \varphi < 1$ is a boundary cell.

The system size is $L_x = 1400$ nm along the global temperature gradient and $L_y = 4800$ nm for the transversal direction. We adopted the grid size 25 nm. Starting from properly chosen initial temperature distribution, the time development of $f(\vec{k}, \vec{r}, t)$ is traced with Eq. (1). Data analysis for the local temperature and the local phonon flux is done for the steady state, which is reached typically within 1 ns.

2.2. Electric Conductivity

Since the typical MFP of electrons is much shorter than that of phonons in Si crystal, we analyse the electric conductivity using a two-dimensional square network of Ohmic resistance [5]. Given the electrostatic potential difference between $x = 0$ and L_x, the local potential and the local current at the steady state is calculated by iteration, and the effective electric conductivity σ is evaluated.

2.3. Porous Film Modelling

We fabricated various types of two-dimensional porous film model by utilizing molecular dynamics (MD) simulation of two-dimensional particles with specified diameter D. As show in Table 1, we prepared three "monodisperse" systems ($D =$ 800, 400, and 200 nm) and their mixture as "polydisperse" ones; note that $D =$ 400 nm roughly corresponds to the

Table 1: Simulated systems of nano-porous thin film.

	Symbol	Number of particles			Mean diameter D_{mean} [nm]	Porosity ϕ	Tortuosity k mean of five samples
		800 nm	400 nm	200 nm			
monodisperse	Mono-800	14	–	–	800	0.0799 - 0.1334	1.317
	Mono-400	–	56	–	400	0.0732 - 0.0850	1.221
	Mono-200	–	–	224	200	0.0631 - 0.0526	1.131
polydisperse	Poly-(6,16,64)	6	16	64	514.3	0.0200 - 0.0317	1.070
	Poly-(4,24,64)	4	24	64	457.1	0.0336 - 0.0493	1.121
	Poly-(2,32,64)	2	32	64	400.0	0.0705 - 0.0917	1.208
	Poly-(0,40,64)	0	40	64	342.9	0.1005 - 0.1475	1.379

relevant phonon mean free path. The MD simulations were done with the LAMMPS [6] package; the Lennard-Jones model was adopted for the interparticle potential, which brings some variations in interparticle distance, leading to some variations of porosity ϕ depending on configurations. The tortuosity, which is an important transport property of porous materials, is evaluated as the inverse ratio of electric conductivity.

3. Results and Discussion

For each model in Table 1, we prepared five samples with different particle configurations. Examples of local phonon temperature at steady state are shown as a colour map in Figure 2, which indicate that the "neck" region between particles effectively hinders phonon transport.

The effective thermal conductivity κ is evaluated from the obtained phonon flux q_x, as

$$q_x = \kappa \frac{T_H - T_L}{L_x} \tag{4}$$

where T_H and T_L are the temperature of each thermal reservoir (hot and cool), respectively. The non-dimensional figure of merit is defined [1] as

$$ZT = \frac{S^2 \sigma T}{\kappa} \tag{5}$$

where S is the Seebeck coefficient (assumed to be a material constant) and T is the mean temperature. The results are summarized in Figure 3, where the relative values to those for a monolithic sample are indicated. While the electric conductivity seems to be a unique function of porosity ϕ because of its Ohmic nature; phonon transport is more suppressed

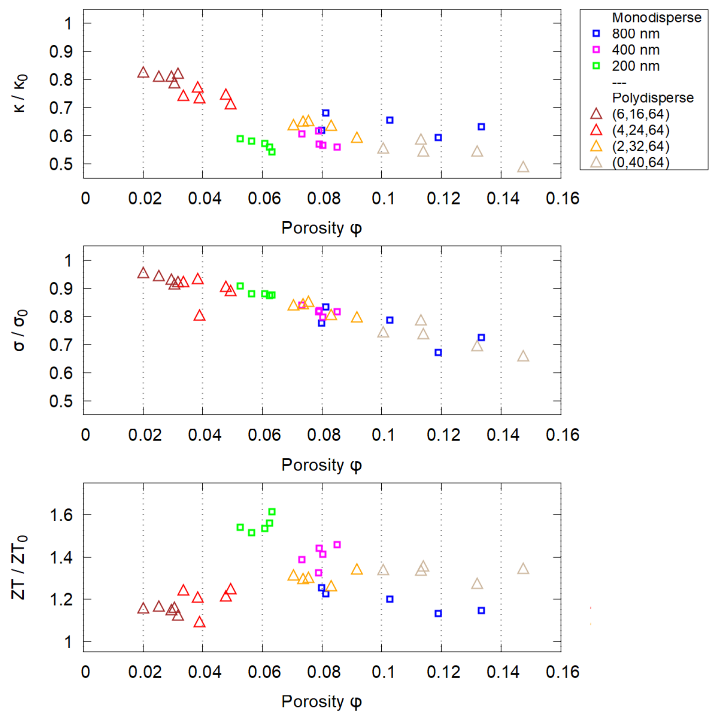
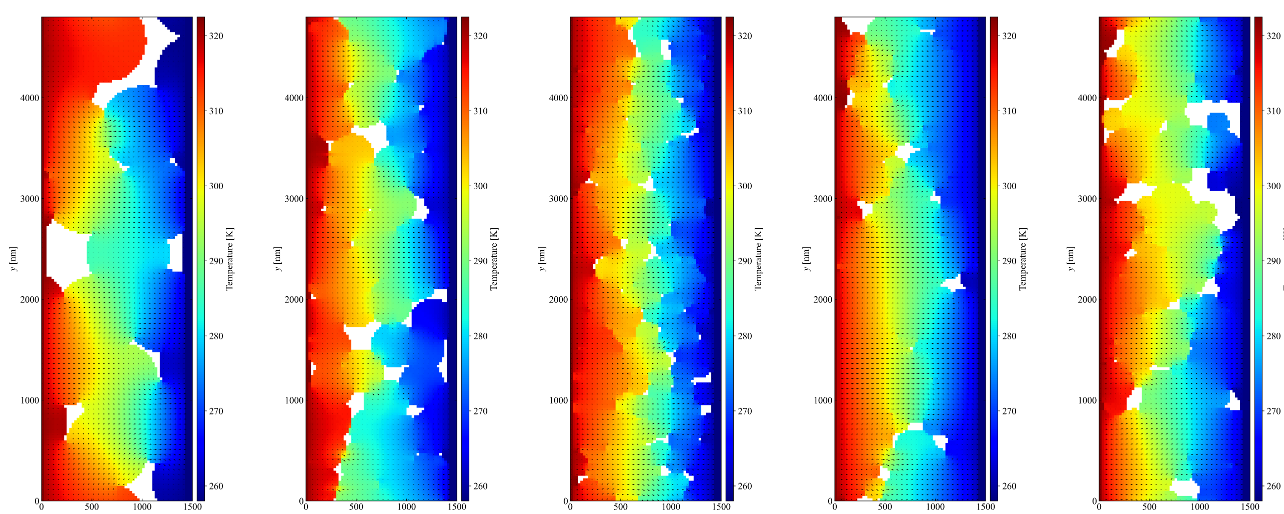


Fig. 3: Evaluated thermal conductivity κ, electric conductivity σ, and figure of merit ZT; relative values to the structure-less film.

in films consisting of smaller particles. Among the systems investigated here, the porous film consisting of the smallest particles ($D = 200$ nm) gives the best performance, although the porosity is not so large.

4. Conclusion



(a) Mono-800 (b) Mono-400 (c) Mono-200 (d) Poly-(4,24,64) (e) Poly-(0,40,64)

Fig. 2: Examples of obtained temperature distribution (colour map) and phonon flux (arrows) in steady state.

We studied the thermal and electrical conductions in modelled porous thin films. The phonon transport investigated based on BTE is much affected by the characteristic length scale of pores while the electric conductivity is solely determined by the porosity. These findings can lead to structural optimization of thermoelectric conversion of porous materials.

References

[1] G. Chen, *Nanoscale Energy Transport and Conversion*. Oxford University Press, 2005

[2] S. Volz1, J. Ordonez-Miranda1, A. Shchepetov, M. Prunnila, J. Ahopelto, T. Pezeril, G. Vaudel, V. Gusev, P. Ruello, E. Weig, M. Schubert, M. Hettich, M. Grossman, T. Dekorsy, F. Alzina, B. Graczykowski, E. Chavez-Angel, J. Reparaz, M. Wagner, C. Sotomayor-Torres, S. Xiong, S. Neogi, and D. Donadio, "Nanophononics: State of the art and perspectives," *Eur. Phys. J*. B, Vol. 89, 15, 2016.

[3] Z. Wang, J. Alaniz, W. Jang, and J. Garay, and C. Dames, "Thermal Conductivity of Nanocrystalline Silicon: Importance of Grain Size and Frequency-Dependent Mean Free Paths," *Nano Lett.*, Vol. 11, pp. 2206-2213, 2011.

[4] Y. Takahara, M. Matsumoto, M. Hanaoka, and M. Iwakawa, "Phonon transport simulation with an extended VOF scheme for nano-structured thin film," *Appl. Phys. Lett*., Vol. 124, 172204, 2024.

[5] M. Sato, Y. Takahara, M. Matsumoto, N. Kajinami, M. Hanaoka, and M. Iwakawa, "Thermal control of thin films with nano structure," in *Proc. 9th Eurotherm Conf.*, Bled, Slovenia, 2024; *J. Phys.: Conf. Ser.*, Vol. 2766, 012206, 2024.

[6] Web page, https://www.lammps.org/