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Numerical investigation of thermodynamic properties in 2D porous silicon photonic crystals integrated in thermophotovoltaic energy conversion system

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ABSTRACT

The prediction of thermodynamic properties performance in porous silicon (pSi) photonic crystals (PhCs) was studied for enhancement of light conversion into different types of energy based thermophotovoltaic energy conversion system. The unit-cell for 2D square and triangular lattices of circular air holes were formulated and solved using plane wave expansion (PWE) method. This was used to investigate the thermodynamic properties and the effect of lattice dynamic on these properties at different porosities in silicon PhCs; which are regarded as isolated and non-interacting particles systems. This was achieved by connecting density of states (DOS) and thermodynamic quantities as described in statistical physics. It revealed that irrespective of lattice type, increasing porosity ensued a decline in thermodynamic properties. Novel insights and theoretical concepts that could be integrated in thermophotovoltaic system were revealed. Regarding the square lattice, the optimum value of these properties except the free energy was obtained at $R/a = 0.30$ for 20% and 50% porosities, and at $R/a = 0.25$ for 80% porosity. Regardless of the porosity, the optimum value for the triangular lattice was found at $R/a = 0.25$. These characteristics have attempted to provide contributions with regards to the selection of the appropriate design for PhC in order to achieve high efficiency conversion.

1. Introduction

Recent strides in silicon technology has brought about porous silicon (pSi); a prodigious material which has been introduced in various scientific and engineering fields including photonics and energy technologies [1–11]. Thermal radiation from photonic crystal (PhC); often referred as complex electromagnetic structures, has recently attracted the attention of several researchers [12–18]. Lin et al. indicated that the thermal radiation from metallic PhCs probably exceeds that of a blackbody in free space [15]. The effect of thermal oxidation and oxide etching on silicon PhCs of triangular lattice has been studied. Using plane wave expansion (PWE) technique, Thitsa & Sacharia [19], modeled the latter and proposed advantageous processes for tuning the photonic band gap and defect frequency. Indeed, the knowledge on the propagation of electromagnetic fields in PhCs, analytical and numerical methods are available. These methods allow the access to quantities deemed inaccessible by experimental measurements but which can be necessary for understanding the behavior of PhCs. Among these different methods, the PWE remains the most commonly used in studying the band structure of PhCs and has been employed by different authors in the investigation of PhCs [20–24]. Currently, there are numerous proposed applications relating to pSi based PhCs. This is largely due to their ability to control light propagation within them as reported in Ref. [5]. Luo et al. presented a classical simulation of equilibrium thermal emissivity from dispersive lossy PhCs [25]. They indicated the potential usefulness of PhCs in incandescent lighting and thermal photovoltaic applications. Furthermore, a basis for manipulating the thermal emission and absorption of radiation in complex photonic structures and the design of novel solar cell devices has been reported by Florescu et al. [26]. These authors revealed that controlling the thermal

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Table 1
Refractive index and dielectric constant versus porosity in Bruggeman model [41,42].

Porosity (%)	Refractive index (n_{Si})	Dielectric constant (ε_{Si})
Bulk	3.47	12.04
10	3.23	10.43
20	2.98	8.88
30	2.72	7.40
50	2.14	4.58
70	1.56	2.43
80	1.32	1.74
90	1.12	1.25

emission and absorption of radiation in a PhCs enables the realization of high-efficiency solar cells. Florescu et al. in another study, analyzed the origin of thermal radiation enhancement and suppression inside PhCs as a prerequisite for the understanding the thermal radiation properties of finite PhCs [27]. Moreover, Gesemann et al. presented measurements of the thermal emission properties of 2D and 3D silicon PhCs which depended on substrate heating (resistively and passively) with an aluminum hotplate [28]. A decrease in the averaged energy of 2D PhCs based on bulk and pSi materials was revealed by Szabo et al. who applied finite differential time domain (FDTD) method in calculating wave propagation [29]. Tong et al. indicated that both dispersion characteristic analysis and numerical simulation of field patterns can verify the effective phase indexes of 2D triangular PhCs with dielectric rods in air background [30].

Currently, applications of thermal light sources through PhCs are being explored, mainly in the field of thermophotovoltaic power conversion. However, the demands of high-operating temperatures inevitably leads to nano and microscopic material degradation which are challenging [31–35]. However, the estimate of optimum thermodynamic properties of materials is the emphasis of solid-state knowledge and industrial research which is applying in several modern technologies at high temperature as well as low temperature configuration [36–40]. Other relevant works and their findings are summarized in Table 2.

Based on existing knowledge, thermodynamics is a subject of great generality which is applicable to systems of elaborate

Table 2
List of relevant research works and key findings.

Authors	Type of research	Type of devices	Key findings
Schilling & Scherer [8]	Experimental	3D PhC	Reflection measurements along different directions indicate the onset of the 3D bandgap at low frequencies for an extended fabricated structure.
Bicer et al. [40]	Numerical	Photovoltaic cell	The PV generator-photo current generation process has the highest exergy destruction rate among the sub-processes.
Shimizu et al. [34]	Experimental	Periodic microcavities	The effect of spectrally selective property is appeared as increasing of the temperature comparing with the black painted sample.
Rinnerbauer et al [31]	Numerical & Experimental	2D PhC	The efficiency of selective emitters based on 2D PhCs in refractory metals.
Mogami et al. [33]	Experimental	Optical waveguide devices	Their Si photonics platform is very useful for optical multi-applications.
Florescu et al. [26]	Numerical & Experimental	Solar cell	Strong enhancement of the conversion efficiency of solar cell devices without using concentrators was achieved by PhC.
Latella et al. [57]	Numerical	Energy conversion devices	The maximum work flux that can be obtained from near-field radiation is almost two orders of magnitude more than the corresponding for blackbody radiation if one considers sources of hexagonal boron nitride. For other materials with a lower resonance frequency, e.g., silicon carbide, the maximum work flux is even higher.
Wang et al. [13]	Numerical	2D & 3D PhCs	In 2D, using van Hove singularity in the DOS, the angle-integrated light trapping absorption enhancement factor can exceed the conventional limit over a substantial bandwidth. In 3D, it is more difficult to use PhCs to overcome the conventional limit.
Recio-Sanchez et al [42]	Numerical	2D & 3D PhCs	These structures are very promising candidates for the development of low-cost photonic devices.
Kordas et al. [61]	Numerical & Experimental	pSi Layer	Normal optical dispersion on the contrary to the anomalous dispersion obtained using the envelope method.
Fu et al. [7]	Numerical	2D PhC	The operation of logic gates does not require high power excitation.
Johnson et al. [12]	Numerical & Experimental	PhC	Enhancement of Er^{3+} emission intensity is observed for the 550-nm transition, with lower enhancement factors seen for longer wavelengths.
Flores & Palma-Chilla [38]	Numerical	Dual & direct systems	Entropies correlated being a basic tool to attach thermodynamically both categories of systems. It is explicitly showed that the Dual has negative temperatures and positive pressures.
Chan et al. [17]	Numerical	2D PhC	The ability to design thermal emission could well find uses in thermophotovoltaic systems and defense applications.
Gesemann et al [28]	Numerical & Experimental	2D & 3D PhCs	It turned out that for the in-plane 2D PhC and out-of-plane 3D PhC emission a photonic stop gap effect is visible. For the out-of-plane 2D PhC emission, no photonic bandgap effect is observable but instead strong silicon oxide emission from native oxide inside the pores of silicon are observable.
Hu et al. [11]	Numerical & Experimental	Silicon photovoltaic	This study provides a basic understanding of thermal performances, such as the temperature field and heat transfer coefficient.
Florescu et al. [27]	Numerical	2D PhC	The spectral energy density, the spectral intensity, and the spectral hemispherical power are only limited by the total number of available photonic states and their propagation characteristics. The central quantity that determines these thermal radiation characteristics is the area of the isofrequency surfaces and not the photonic density of states as it is generally assumed.
Lourek & Tribeche [54]	Numerical	Blackbody	The reexamination of the thermodynamic properties of the blackbody radiation shows that it emits more energy with an increase of the value of $\lvert\kappa\rvert$ in comparison with the standard Planck radiation law. Moreover, the effects of the deformed Kaniadakis statistics are shown to be more appreciable for high temperatures.
Lin et al. [15]	Experimental	3D PhC	A 3D tungsten PhC sample is thermally excited and exhibits emission at a narrow band. The sharp emission is experimentally shown to exceed the free-space Planck radiation. It is proposed that an enhanced DOS associated with the propagating electromagnetic Bloch waves is responsible for the observed effect.