Spectral Control of Thermal Radiation using Rectangular Micro-Cavities on Emitter-Surface for Thermophotovoltaic Generation of Electricity*

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Abstract
Spectral control of thermal radiation emitted from rectangular micro-cavities made on a metal surface was investigated through numerical simulation and experiment. In the numerical simulation, thermal radiation from solid surface was dealt as hemispherical emission from point sources, and the Maxwell’s equations were solved using the cubic interpolated propagation method. It was demonstrated that spherical waves emitted from inside of a cavity were spectrally selected, and that the emittance could be increased around the wavelength corresponding to the standard mode of cavity resonance. Furthermore, in experiment using rectangular micro-cavities (0.5x0.5x0.5 µm$^3$) made periodically on Ni specularly-polished surface, spectral emittance was measured in the near-infrared region. The experimental results disclosed that the emissive power only in the range of shorter wavelength than 1.2 µm was increased by the micro-cavities that played a role of a wave guide to produce cutoff effect clearly.

Key words: Thermal Radiation, Spectral Control, Surface Micro-Structure, Emission Model, Measurement of Emittance

1. Introduction
Thermophotovoltaic (TPV) generation of electricity is one of the promising techniques to utilize thermal energy. In TPV systems, radiation energy emitted from any kind of heat source is directly converted into electricity by a TPV cell. Typically, a TPV cell has a very narrow bandwidth for an active range of wavelength. A GaSb TPV cell, for example, exhibits high quantum efficiency over the wavelength range from 0.8 to 1.8 µm, that is, thermal radiation with those wavelengths is converted into electricity with a conversion efficiency of about 30% [1]. Therefore, spectral control of thermal radiation to conform the band-gap of cell is the core issue for achieving high energy conversion efficiency in TPV systems.

To date, some types of spectrally selective emitter have been proposed [2]. Among those, rare-earth oxide materials possess a highly selective emittance. However, their characteristic wavelengths are confined only in narrow bandwidths, and such materials are so fragile that a durability issue comes up [3]. On the other hand, a micro-structured emitter can be fabricated by making use of various metals, and its spectral property can be controlled by the surface structure. Hence, for application to TPV systems, the latter way of spectral control is useful in designing a proper emitter spectrally matching to each TPV cell,
such as GaSb (< 1.8 \mu m), GaInSb (< 2.5 \mu m) or InPAsSb (< 3.5 \mu m) \[4\].

In the field of thermal radiation, effect of surface micro-structure on emissive property is not a new finding. Directional emission from grooved surface is well-known and spectral characteristics have also been reported \[5-7\]. Strong directionality and spectral property of coherent thermal emission due to coupling with surface waves was reported \[8\]. Whereas these studies were focused on one-dimensional surface-relief gratings, rectangular micro-cavities with an aperture area of 5.0x5.0 \mu m^2, were made on a Si surface, and then, were Cr-coated \[9\]. It was demonstrated that its emittance was enhanced in the wavelength range shorter than 10 \mu m in measurement at around 760 K. After this experiment, the same type of surface micro-cavities with an aperture area of 0.8x0.8 \mu m^2 was fabricated on single crystalline substrates made of tungsten, and amplification of emittance in the wavelength range of less than about 1.5 \mu m was demonstrated \[10\]. These experiments definitely showed possibility of spectral control by using surface micro-structure in the near-infrared to infrared region. Furthermore, it was proposed that characteristic wavelength of emittance modified by surface structure could be explained by resonant modes of electromagnetic waves in a rectangular cavity. The result of this calculation predicted peaks in the spectra of emittance well. And there is no peak of emittance in the longer wavelength range than a wavelength corresponding to a normal mode of resonance. However, emittance is magnified also in the long wavelength region nearly twice the value of specularly-polished surface in all their experimental results. This is not favorable for application to TPV systems because energy of emitted waves not matching to the bandgap of a TPV cell is not converted into electricity but dissipates as thermal energy. Ideally, emittance in the long wavelength region remains to be the same as that of polished surface which is intrinsic property of material, and enhance it as great as possible up to unity at resonant wavelengths. In order to realize optimum design of an emitter, it is required that the phenomenon of thermal radiation emitted from micro-structured surface is well-understood and the method of predicting emittance is established.

For prediction of spectral property, the rigorous coupled-wave analysis (RCWA) method \[10\] and the finite-difference time-domain (FDTD) method were used \[11\]. These methods are indirect ways for calculation of emissive property. In these simulations, absorptance of surface is calculated from reflectance of plane waves, and then, emittance is obtained assuming it is equal to absorptance on the basis of Kirchhoff’s law \[12\]. Add to that, use of incident plane wave in those indirect methods for periodic structured surface could cause interference due to its coherency which is irrelevant to thermal emission which is considered to be a spherical incoherent wave emitted from sources in random thermal motion. Recently, experimental and numerical comparison of emittance and absorptance was conducted for the micro-structured surface, and difficulty of indirect measurement of emittance was reported \[13\]. Therefore, a direct and primitive model of thermal emission is required, and it could give more intuitive understanding of thermal scientific phenomenon and be useful for farther development of thermal engineering.

Although there have been tremendous progress recently in the field of micromachining, it is still difficult to fabricate micro-structure on a metal surface, especially making it in large area enough to be used as an emitter. Experimental studies referred to above also reported roughness of walls in rectangular cavities and deterioration of micro-structure after heating \[9,10\]. Thus, there are many remaining problems to be handled concerning fabrication and treatment in the process of usage. Furthermore, it is hard to obtain high accuracy of emittance in measurement, which is mainly due to difficulty of detecting surface temperature with a high degree of accuracy, and radiation thermometer was used to detect surface temperature of an emitter in the previous studies \[9,10\]. Measurement of surface temperature of a metal emitter can be conducted more precisely by using thermocouple welded on its surface than using a radiation thermometer. Hence, further
experimental verification of amplification of emittance with due care is profitable.

In the present study, spectrally selective property of micro-structured surface is investigated through numerical simulation of electromagnetic waves, in which 3D hemispherical emission model is proposed and the Maxwell’s equations are solved rigorously. And periodic micro-cavities with aperture area of 0.5x0.5 μm² were fabricated on a Ni specularly-polished substrate. The size of cavities are determined by taking into consideration an application to TPV systems, and that it is smaller than previously reported ones in order to demonstrate that this spectral control method can be applied to a wide range of spectrum from wavelength shorter than 1.1 μm using Si-base cells to that shorter than 3.5 μm using InPAsSh-base cells, in thermal radiation. Then, enhancement of emittance by the micro-cavities has been confirmed through experiment.

NOMENCLATURE

\[ A \] area, m²
\[ B \] magnetic field, T
\[ c \] speed of light in vacuum, m/s
\[ E \] electric field, V/m
\[ J \] current density, A/m²
\[ L \] size of cavity, m
\[ S \] absolute value of Poynting vector, W/m²
\[ t \] time, s
\[ x, y, z \] space coordinates, m
\[ (\text{\textprime}) \] time-averaged value

Greek symbols
\[ \varepsilon \] emittance
\[ \varepsilon_0 \] permittivity in vacuum, C²/Nm²
\[ \varepsilon_{ijk} \] permutation symbol
\[ \Lambda \] periodic interval of cavities, m
\[ \lambda \] wavelength, μm
\[ \mu_0 \] permeability in vacuum, N/A²

Subscripts and superscripts
* non-dimensional value
\[ i, j, k \] indices of space components
\[ m, n, l \] integers
\[ \text{flat} \] specularly-polished flat surface
\[ \text{ms} \] micro-structured surface
\[ p \] plane surface

2. Numerical Simulation on Thermal Radiation

2.1 Hemispherical Emission Model

Mechanisms of emission of thermal radiation from solid are thermal vibration of atoms and bound electron transition [12]. Though these mechanisms are quite different as physical phenomena, electromagnetic waves emitted due to both mechanisms can be considered to be waves propagating spherically. In the current study, thermal radiation from solid surface is modeled as hemispherical emission from point sources. Point sources are expressed by current density terms existing on the surface in the Maxwell’s equations.
In solving the Maxwell's equations, the cubic interpolated propagation (CIP) method [14-17] is used. Although the CIP method has been applied successfully to various kinds of fluid simulation, there are not so many examples of application to electromagnetic field analysis. On the other hand, the FDTD method is widely used in the field of numerical simulation of electromagnetic field, and a lot of numerical techniques have been developed and available [18]. However, there are some advantages of using the CIP method in the simulation of thermal emission. First, numerical dispersion can be greatly suppressed in comparison to the case of the FDTD method. This characteristic is quite useful because accuracy of calculation is maintained in a wide range of wavelength with the same numerical grid configuration. Second, free boundary condition is satisfied automatically for all outgoing waves without dependence of frequency and angle of incidence to boundaries, so there is no need of treatment such as an absorbing boundary condition used in the FDTD method. This feature is useful especially in the simulation of incoherent emission from solid surface. In this case, periodic boundary condition can not be applied, so all boundaries except emitter surface are needed to be set as free boundaries which express infinitely extended space.

Reformulation of the Maxwell’s equations into formulae solved by using the CIP method is straightforward. First, equations (1) and (2) in vacuum are normalized for convenience.

\[
\frac{\partial E_i^*}{\partial t} - c^* \left( \frac{\partial B_j^*}{\partial x_j} + \frac{\partial B_j^*}{\partial x_i} \right) = -J_i^* \quad (3)
\]

\[
\frac{\partial B_i^*}{\partial t} + c^* \left( \frac{\partial E_j^*}{\partial x_j} + \frac{\partial E_j^*}{\partial x_i} \right) = 0 \quad (4)
\]

Herein, the subscripts denote space component, and asterisks show normalized values defined as below.

\[
x_i^* = \frac{x_i}{X}, \quad t^* = \frac{t \cdot c}{X}, \quad E_i^* = \frac{E_i}{E_0}, \quad B_i^* = \frac{c \cdot B_i}{E_0}, \quad J_i^* = \frac{J_i}{c \cdot \mu_0 \cdot E_0}, \quad c^* = 1
\]

In these definitions, \(X\) is characteristic length and \(E_0\) is characteristic magnitude of electric field, and these values are introduced for normalization. A non-dimensional velocity is remained explicitly in the following equation in order to express advection formulae clearly. Next, source terms in the right-hand side in equation (3) are eliminated and time integrals of them are conducted separately. This splitting of non-advection terms gives symmetrical reformulation of the Maxwell’s equations. Then, equations (3) and (4) with no current density term are expressed in one form.

\[
\frac{\partial W}{\partial t} + A_x \frac{\partial W}{\partial x} + A_y \frac{\partial W}{\partial y} + A_z \frac{\partial W}{\partial z} = 0
\]

where \(W = (E_x^*, E_y^*, E_z^*, B_x^*, B_y^*, B_z^*)^T\),

\[
A_x = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & -c^* \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -c^* & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & -c^* & 0 & 0 & 0 & 0 \\
c^* & 0 & 0 & 0 & 0 & 0
\end{pmatrix}, \quad A_y = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & c^* \\
0 & 0 & 0 & c^* & 0 & 0 \\
0 & 0 & c^* & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
-c^* & 0 & 0 & 0 & 0 & 0
\end{pmatrix}, \quad A_z = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]
Calculation is conducted separately in $x$, $y$ and $z$ directions. After directional splitting of equation (5), each tensor is diagonalized utilizing eigenvalues of it. Then, simple advection equations for three directions are obtained. Values of electric and magnetic fields are renewed three times within one time step. The details are described in Ref. [16]. Finally, the Maxwell’s equations are solved by using twelve advection equations and three non-advection equations.

$$\left( \frac{\partial}{\partial t} + c^* \frac{\partial}{\partial x_i} \right) (E_j^* \pm B_i^*) = 0$$

(6)

$$\frac{\partial E_i^*}{\partial t} + J_i^* = 0$$

(7)

Every field component is calculated on the same numerical grid. In advection calculation process, each interval value of field components between numerical grids is interpolated by cubic polynomial. Partial derivatives of each component of electric and magnetic fields with respect to space variables are also calculated on each grid in order to determine the shape of cubic polynomial. Positioning of field vector components are different from the Yee space lattice of the FDTD method in which electric field and magnetic field are located in staggered position. Therefore, Poynting vector is easily obtained on each grid in the CIP method. Figure 1 shows contour surfaces of absolute value of Poynting vector, $S$, in a numerical domain. In this case, a point emitting source is placed on the bottom surface. The bottom surface is assumed to be a conductor, while other boundaries are free boundaries. Electric field is polarized depending on the direction of given current density. It should be noted in these figures that emitted spherical waves are passing through free boundaries without deformation, and which means that characteristic of the CIP method is successfully implemented. Furthermore, electric fields emitted from current densities having orthogonal components are superposed for modeling of thermal emission which has no special polarization. The 3D numerical simulation code developed here was validated also by energy distribution of dipole emission in free space and reflection of wave at solid surface.

![Fig.1 Hemispherical energy distribution emitted from a point source on a conductor surface. Two figures show different contour surfaces of $S$. Outgoing spherical waves are passing through free boundaries without deformation.](image)
2.2 Calculation Condition

Figure 2 shows schematic diagram of the micro-cavity configuration of numerical domain. The emitting surface, where point sources are placed, is divided into three parts, i.e., I, the bottom of cavity, II, the sidewalls of cavity and III, the outside surface. Numerical simulation is conducted assuming that micro-cavity has perfectly conducting surface, that is, \( \mathbf{E} = 0 \) and \( \mathbf{B} = 0 \) inside the material. Hence the boundary conditions are that the components of \( \mathbf{E} \) parallel to the walls and the components of \( \mathbf{B} \) perpendicular to the walls are zero. Basically, from Kirchhoff’s law, the perfectly conducting surface does not emit radiation since the emissivity is truly zero; that is, the reflectivity is unity. Therefore, it is assumed that only a numerical grid assigned as an emitting-source point has a finite emissivity while the all other surfaces satisfy the perfectly-conducting condition. The numerical calculation is performed for each emitting-source point individually, and then, added over all numerical results.

As mentioned above, emission of thermal radiation is caused by random vibrational-rotational motions in the atomic lattice of material. In this case, each electric dipole as an emitting-source has an individual frequency, phase and amplitude. As a result, it is assumed that emitting sources don’t interfere with each other. On the other hand, radiation emitted from a single emitting-source will interfere with multi-reflected radiation emitted from the same source since it propagates spherically in the cavity. In the present calculation, areas of I and III are fixed (i.e., \( L_x = L_y = L_z = 1.5L \)) and effect of cavity depth, \( L_z \), is of interest. An aperture area of rectangular cavity is divided by 33x33 grids uniformly, and also grids are set in the \( z \) direction. Time interval is set by taking Courant condition into consideration. Spectral emissive power is estimated by time averaged absolute value of Poynting vector in the normal direction of the cavity and distance \( L \) above the surface of the region III. Under these conditions, resonant wavelengths are given by,

\[
\lambda_{res} = \frac{2}{\sqrt{\left(\frac{m}{L_x}\right)^2 + \left(\frac{n}{L_y}\right)^2 + \left(\frac{2l+1}{2L_z}\right)^2}} \tag{8}
\]

where \( m, n \) are integers which are not simultaneously equal to zero, and \( l \) is also an integer. From the theory of an infinitely-long rectangular wave guide, the wavelength corresponding to the cutoff frequency is \( \lambda = 2L \). Thus, waves with longer wavelength than \( 2L \) are not propagating in a rectangular cavity and going out of it. It should be noted here that these analytic solution of the Maxwell’s equations are obtained under the condition that boundaries are all assumed to be perfect conductor and that steady state are formed without wave source being taken into consideration [19]. From this point of view, it is unknown
whether spherical waves emitted from inside of a rectangular cavity show spectral property described above analytic solution. Therefore, in this study, solid boundary is assumed to be perfectly conducting surface, and behavior of spherical waves are investigated.

2.3 Numerical Results and Discussion

Figure 3 shows the non-dimensional spectral emissive power which is normalized by that of the plane surface as follows.

\[
\frac{\langle S' \rangle_{\text{Total}}}{\langle S' \rangle_{\text{p}}} = \frac{\langle S' \rangle_{\text{I}}}{\langle S' \rangle_{\text{p}}} + \frac{\langle S' \rangle_{\text{II}}}{\langle S' \rangle_{\text{p}}} + \frac{\langle S' \rangle_{\text{III}}}{\langle S' \rangle_{\text{p}}} \quad (9)
\]

In this case, the ratio of the cavity-depth to the cavity-size is \(L_z/L=4/3\). In this figure, in addition to the total power, its components emitted from three different regions I, II and III are also shown. In the total spectral emissive power, there exists a large peak around \(\lambda/L=1.7\) which is close to the resonant mode of \(\lambda_{100}\sim 1.87L\) and cutoff of long-wavelength radiation (\(\lambda/L >2\)) due to wave guide effect can be seen. Among the spectrum for three components, the cutoff effect is remarkable for emissive power from region I.

Emission from region II is dominant because surface area \(A_{\text{II}}\) is larger than other areas (\(A_{\text{II}}/A_{\text{I}} >5\)). However, emitted waves from the inside of cavity should be attenuated. To explain this, emission from the region II in the case of \(L_z/L=2\) is indicated in detail as follows.

Figures 4 and 5 show locations of emission sources on the region II and the normalized spectral power emitted from each source point, respectively. The cutoff effect becomes remarkably large as emission source is located at deeper position in the cavity, and emission from \(z=z_6\), the shallowest point, is not reduced significantly. On the other hand, at the wavelength corresponding to the cavity resonance, emissive powers from \(z=z_3, z_4\), the middle of the cavity, show large quantity. Therefore, at the resonant wavelength, the emissive power becomes higher as the area of the region II becomes larger. Over the cutoff wavelength, emissive power is almost due to the emission from the sources located at shallow points.

Figure 6 shows the normalized total emissive power defined by equation (9) for \(L_z/L\) of 2/3, 1, 4/3 and 2. As \(L_z\) is enlarged, the spectral emissive power shows the more notable peak around the wavelength corresponding to the normal mode of the cavity resonance. Simultaneously, the peak wavelength is shifted to longer range, and this characteristic is predicted by equation (8). On the other hand, in the long-wavelength region, the emissive power takes almost the same value despite enlargement of the cavity depth. Furthermore, at
wavelengths corresponding to higher modes, emissive powers are not so amplified as at the normal mode.

It is demonstrated that making micro-structures on the solid surface indicates possibility of spectral control of thermal radiation. In this simulation, radiation properties of the emitter, such as the complex refractive index, are not taken into account. Consequently, there is no absorption of energy at the walls in the cavity. Therefore, though absorptance is small in the case of metals, the amplification of emissive power might be reduced slightly in practice.
3. Measurement of Emissive Property

3.1 Preparation of Ni Emitter

Figure 7 shows a photograph and a SEM image of the micro-cavities made on the specularly-polished nickel metal surface. The surface micro-structure was fabricated by means of the photolithography and fast atom beam etching (FAB) techniques. Size of the substrate made of Ni is 25 mm in diameter, and in the center of it rectangular micro-cavities (0.5x0.5x0.5 \(\mu\)m\(^3\)) were made periodically in the area of 2.0x2.0 mm\(^2\). From observation of this micro-structured area, it is clear that this area has strong directional reflective property such as a diffraction grating. However, concerning emission of thermal radiation, characteristic directionality is not reported by measurement in previous research [9]. Therefore, only normal spectral emittance is measured in the present study.

Selection of nickel as an emitter substrate has two advantages. First, thermocouples are easily welded on nickel surface. Measurement of emittance is difficult because emissive power is quite sensitive to surface temperature. From this reason, high accuracy of surface temperature measurement using welded thermocouples is required. Next, emissivity of nickel polished surface is very low in the near infrared region. Therefore, nickel has a high potential of amplification of emittance, in other words, distinct selectivity can be achieved by using micro-structured surface.

3.2 Experimental Setup and Procedure

Figure 8 shows a schematic diagram of optical system for measurement of emissive power. Nickel emitter is placed in the vacuum chamber in order to prevent it from being oxidized. The CO\(_2\) laser (NEOARK, NAL-50D) ray is introduced into the vacuum chamber through a germanium window and zinc-selenide lens and is incident on the back surface of the Ni emitter sample. The sample is heated up to 1052 K. The surface temperature is measured by a pair of armel-cromel thermocouple fixed by welding on the surface. Thermal radiation emitted from the Ni emitter, after traveled through a sapphire window, is focused on the entrance of the spectrometer (Ritsu Applied Optics, MC-10N3G) using a concave mirror and a plane mirror. Then, the spectral emissive power is measured by Si photodiode (Hamamatsu Photonics) in the wavelength range of 0.7 \(\mu\)m to 1.1 \(\mu\)m, and thermopile detector (Ishizuka electronics, MIR-100C) in longer than 1.1 \(\mu\)m.

![Figure 7](image-url)  
**Fig. 7**  A photograph of a Ni emitter and a SEM image of rectangular cavities (0.5x 0.5x 0.5 \(\mu\)m\(^3\)) on the specularly-polished surface.
In this experiment, the emitter sample has the micro-structured surface only in the small square area of 2.0x2.0 mm². In order to detect a signal for emissive power from such a small area, an aperture of 4.0x4.0 mm² is set at the entrance of spectrometer; where intensities of thermal radiation emitted from both micro-cavities- and non-cavity-areas are superimposed; where the signal intensity is expressed as $V_{\text{ms}} + V_{\text{flat}}$. In addition, thermal radiation emitted from flat Ni surface is also measured; where the signal intensity is expressed as $V_{\text{flat}}$. As a result, the normal spectral emittance is estimated as follows.

$$\varepsilon_{\text{ms}} = \varepsilon_{\text{flat}} \left( \frac{V_{\text{ms}}}{V_{\text{flat}}} - 3 \right)$$  \hspace{1cm} (10)

Herein, the emittance of polished Ni surface $\varepsilon_{\text{flat}}$ is available from literature [20].

### 3.3 Experimental Results and Discussion

Figure 9 shows normal spectral emittance under the condition of the surface temperature of 1052 K. In the long-wavelength region, the emittance of the micro-cavity surface is much the same as that of the flat surface. The emittance of the micro-cavity surface increases with decreasing wavelength from 1.2 μm, which shows the cutoff effect. Furthermore, the emittance has a peak in the range of the wavelength of 0.85~0.95 μm that is very close to that of the standard mode of micro-cavity, i.e., 0.894 μm estimated from equation (8).

Herein, the wavelength of $\lambda = 2L$ in the numerical simulation is equivalent to that of 1...
µm in the experiment. The spectral properties of emission of the rectangular micro-cavity surface are modeled using a point emitting-source and perfectly conducting surface from a comparison between Fig.6 and Fig.9 since those trends are much the same quantitatively in wavelength. And the present experimental result indicates possibility of further refinement about magnitude of emittance in emission modeling.

4. Concluding Remarks

The spectral property of emission from the rectangular micro-cavity surface was investigated through 3D numerical simulation assuming the perfect conductor surface and point sources for hemispherical emission and it was demonstrated that spherical waves emitted from the inside of a cavity exhibit spectral selectivity due to multi-reflection. And experiment was conducted using micro-cavities (0.5x0.5x0.5 µm³) fabricated on the polished Ni metal surface. It has been disclosed that this kind of micro-structured surface is very useful for spectral control of emission of thermal radiation from a heated surface. The wavelength at the maximum emittance is controlled by the cavity aperture size. And the sharp cutoff effect is obtained by high aspect ratio of depth to the aperture size, such as two.

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