Correction of errors in:

A Quantum Dot Near-Field Thermophotovoltaic Device

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Abstract & motivation

As the previously made calcuations seem to have fundamental flaws, the revised methods and conclusions are made and drawn in this paper regarding the topic oultined in the subtitle.

With that being said, in the following sections the new methods are described, followed by the calculations using them, and at last, the new results are evaluated in comparison with previous ones.

The aim of the paper summarized is to provide valid fundations for the conclusions drawn in the previous study, originally describing the device.

Methods

In order to calculate the efficiency of the previously described device, the following equasion has to be utilised [5]:

$$\eta = \frac{P_{el}}{P_{rad}} = \frac{FF * I_{ph} * V_{oc}}{P_{rad}}$$

where η is the desired efficiency, $P_{el} = FF * I_{ph} * V_{oc}$ is the maximum output electric power, P_{rad} is the total thermally radiated power by the heat source, FF is the fill factor, I_{ph} is the photogeneration current and V_{oc} is the open-circuit voltage of the PV cell while being illuminated by the heat source. First, the photogeneration current has to be found for further calcualtions, which can be done by [5]:

$$I_{ph} = e \int_{\frac{E_g}{\hbar}}^{\infty} \frac{P_R(T_1, T_2, \omega)}{\hbar\omega}\, d\omega$$

where e is the charge of an electron, P_R is the frequency distribution of the exchanged radiative power, $\hbar$ is the reduced Planck's constant and ω is the angular frequency of the emitted photons. It shall be noted, that as the dimension of the current also suggests, which is $\frac{C}{s}$, the integral part will have to yield the number of electron-hole pairs generated during a given timeframe, which is also why the beginning of the integration is at $\frac{E_g}{\hbar} = \omega_g$, the angular frequency corresponding to photons of the PV's bandgap energy. Now that this recognition is made, the P_R function requires further examination.

The heat exchange resulting from the near-field thermal radiation of periodic arrays of objects with arbitrary geometries (QDs in the current scenario), is described by the peridodic

DDA [2], which relates the spectral energy density to the previously mentioned arbitrary emitters emitting into free space. In order to obtain the radiative power spectra, first the energy density has to be found. To do so, the LDOS calculated for periodic QD arrays shall be utilized [7] using the following relation:

$$u(\mathbf{r}, \omega) = p(\mathbf{r}, \omega) * \theta(\omega, T)$$

where $u(\mathbf{r}, \omega)$ is the energy density spectra at an observation distance $\mathbf{r}$ from the plane of the array, $p(\mathbf{r}, \omega)$ is the LDOS spectra at the same distance and $\theta(\omega, T)$ is the frequency distribution of the energy levels of electromagnetic states at a temperature T, derived from the Bose-Einstein distribution, and can be calculated as follows [3]:

$$\theta(\omega, T) = \frac{\hbar\omega}{exp(\hbar\omega/k_B T) - 1}$$

where k_B is the Boltzman's constant and T is the temperature of the source. This allows for the calculation of the spectral energy density.

To obtain the spectral radiative power exchange, the propagation of the thermal energy from the observation point has to be considered first. Considering the c-Si PV cell to be isotropic media, the following dispersion relation could be assumed [6]:

$$\omega(\vec{k}) = c|\vec{k}|$$

where $\omega(\vec{k})$ is the angular frequency at which the wave travels in the direction of the wavevector $\vec{k}$, and c is the speed of light in the given media. This equasion allows for the calculation of a group velocity [1] of $\vec{v_g} = \frac{\partial\omega}{\partial\vec{k}} = \frac{c\vec{k}}{|\vec{k}|}$.

Let's assume, that the wavevector in our case is of the same direction as $\mathbf{r}$, and so the heat propagates into the inner layers of the silicon from all observation points, accross the whole cell. This allows to only use the magnitude of the group velocity vector (which equals c based on our assumptions) for the calculation of the power distribution, in the following way [4]:

$$P_R(\omega) = u(\omega)|\vec{v_g}| = u(\omega)c$$

This allows for the calculation of the photogeneration current, the below given way:

$$I_{ph} = e\int_{\omega_g}^{\infty} \frac{p(\omega)}{exp(\hbar\omega/k_BT) - 1} c\, d\omega$$

Based on this, the fill factor and the open-circuit voltage can be calculated as well in the way the next equasions describe [5]:

$$FF = \left(1 - \frac{1}{\ln\left(\frac{I_{ph}}{I_0}\right)}\right)\left(1 - \frac{\ln\left(\ln\left(\frac{I_{ph}}{I_0}\right)\right)}{\ln\left(\frac{I_{ph}}{I_0}\right)}\right)$$

$$V_{oc} = \frac{k_BT}{e}\ln\left(\frac{I_{ph}}{I_0}\right)$$

where T is the temperature of the PV cell and I_0 is the dark current, which can be calculated by [5]:

$$I_0 = e\left(\frac{n_i^2 D_h}{N_D\sqrt{\tau_h}} + \frac{n_i^2 D_e}{N_A\sqrt{\tau_e}}\right)$$

where n_i is the intrinsic carrier concentration, N_D is the donor, N_A is the acceptor concentration, D_e and D_h are the diffusion constants of the electrons and holes, respectively, and τ_e and τ_h are the electron-hole pair lifetimes in the P-doped and N-doped regions, respectively.

Using the previously described methods, P_{el} can be calculated. To calculate P_{rad} as well, the following equasion shall be utilized [5]:

$$P_{rad} = \int_0^\infty P_R(\omega)\, d\omega = \int_0^\infty \frac{p(\omega)\hbar\omega}{exp(\hbar\omega/k_B T) - 1} c\, d\omega$$

Results

Using the methods described in Sec. 2., the following results were obtained.

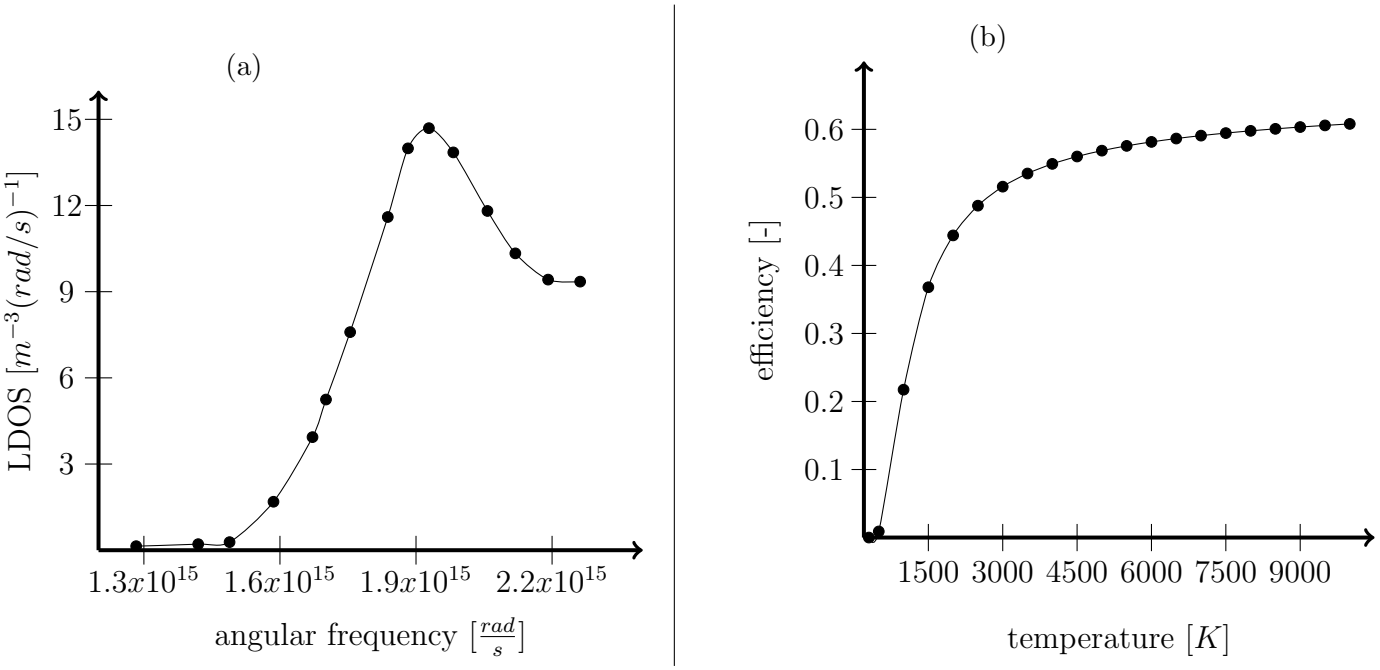

Figure 1: Graphs showing the (a) original spectral LDOS and (b) the obtained efficiency as a function of emitter temperature, at a vacuum gap of 50 nm.

Based on Figure 1 (b), it can be seen, that even though the efficiency reaches significantly higher values than with previous device concepts, it still stays below 50% at temperatures below 2500K, where possible applications may be.

Conclusion

Figure 1 (b) shows, that the previously calculated efficiency is in no correlation with the properly reassessed values, and so the possible implementations of the techology have to be reconsidered, given that the applications mentioned before are not possible based on the new outcomes of the calculations.

References

[1] Abraham Bers. Note on group velocity and energy propagation. *American Journal of Physics*, 68(5):482–484, 05 2000.

[2] Sheila Edalatpour. Near-field thermal emission by periodic arrays. *Physical Review E*, 99(6):063308, 2019.

[3] Sheila Edalatpour and Mathieu Francoeur. The thermal discrete dipole approximation (t-dda) for near-field radiative heat transfer simulations in three-dimensional arbitrary geometries. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 133:364–373, 2014.

[4] D.J. Griffiths. *Introduction to Electrodynamics*. Pearson Education, 2007.

[5] Marine Laroche, Rémi Carminati, and J-J Greffet. Near-field thermophotovoltaic energy conversion. *Journal of applied physics*, 100(6), 2006.

[6] H. Touir and P. Roca i Cabarrocas. Optical dispersion relations for crystalline and microcrystalline silicon. *Phys. Rev. B*, 65:155330, Apr 2002.

[7] Saman Zare and Sheila Edalatpour. The quantum confinement effect on the spectrum of near-field thermal radiation by quantum dots. *Journal of Applied Physics*, 130(1), 2021.