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Quantum Cascade Thermo Photovoltaic Structures for Broadband Energy Conversion

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***Abstract*—A quantum cascade thermo photovoltaic structure is designed to absorb broadband blackbody radiation at 1500 K temperature. A fully quantum mechanical model predicts 35 mV/period open-circuit voltage and 2.94 kA/cm^2 short-circuit current from this structure.**

I. INTRODUCTION

The worldwide increasing demand for electrical energy due to massive technological advancement and the declining reserve of the traditional energy sources are among the major challenges of the time. Emission of CO$_2$, due to burning fossil fuels for producing energy, is causing the world's climate to change adversely. Renewable sources of energy have become an absolute necessity for a sustainable future. Among the renewable energy sources, thermo photovoltaic (TPV) energy conversion devices that absorb the thermal blackbody radiation spectra at 1300 K–2000 K temperature range have not been explored much. Recently, quantum cascade structures based on intersubband transitions have been designed for TPV energy conversion using InGaAs/A1AsSb material system [1]–[3]. Quantum cascade structures employing the intersubband transitions have the potential of tailoring absorption energy and thus increasing efficiency. However, InGaAs/A1AsSb material system has limited capacity in tailoring absorption energy as the X-valley lies at ∼0.75 eV of conduction band offset. Although Refs. [1] and [2] presented an analysis using a semi-classical approach, a much rigorous quantum mechanical approach is required to predict the performances of these devices.

In this work, we design a quantum cascade structure based on GaN/AlN material system for efficient thermo photovoltaic energy conversion. The designed structure absorbs over a broad spectral range around the peak of the blackbody radiation at 1500 K. We develop and implement a fully quantum mechanical model to calculate the open-circuit voltage ($V_{\rm oc}$) and the current-voltage (J-V) relation of the designed TPV structure. We find that the thermo photo-generated $V_{\rm oc}$ across a single stage of the structure is 35 mV and the short-circuit current density ($J_{\rm sc}$) is 2.94 kA/cm^2.

II. STRUCTURE DESIGN

We choose GaN/AlN material system for our structure for its conduction band discontinuity of ∼2 eV so that high energy photons can be absorbed. Additionally, electron scattering rates due to longitudinal optical (LO) phonons in GaN/A1N material system are very fast so that the excited electrons can be collected at the terminals efficiently than InGaAs/A1AsSb material system. The absorption linewidth of nitride material is also large compared to that of the other semiconductor materials of choice. Therefore, photons over a broad energy range can be absorbed in a GaN/A1N material system based on quantum cascade structure, which will result in higher current density.

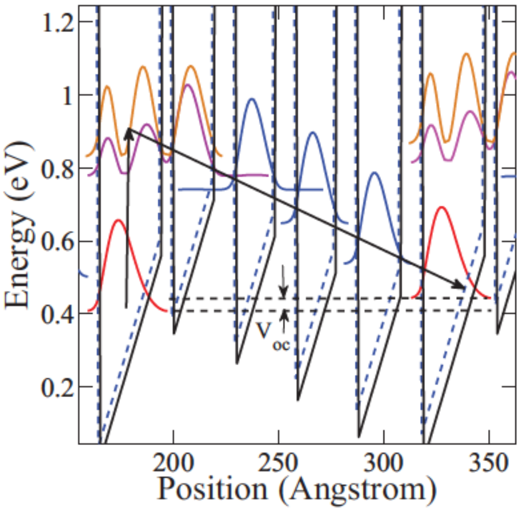

Fig. 1. Conduction band profile of one period of the designed structure. The dashed lines represent change when photo-excited carriers are accumulated at the right side.

The internal electric field generated from the spontaneous and piezoelectric polarization field is taken into account while solving the bandstructure [4], [5]. The conduction band diagram and the relevant moduli-squared wavefunctions of the designed structure are shown in Fig. 1. The well and barrier thicknesses of one period are, in Angstrom, 10/**30**/5/20/10/19/10/19/10/21 starting with an AlN layer. The layer thickness with the bold number is the active region quantum well, which is n-type doped with a density of 5×10^{17} cm^{-3}. The designed structure has two upper transition states so that it can absorb blackbody energy over a broad spectral range. The relaxation path of the excited electrons is designed as a stair case of LO phonon resonance energies. The excited electrons relax through three LO phonon emission steps in only 4.5 ps, which is faster than that in similar structures in Ref. [1].

III. ABSORPTION SPECTRUM

The spectrum of absorption can be calculated by [1]

$$\alpha_{2D}(\hbar\omega) = \sum_{i\in\mathrm{lm}}\sum_{j\in\mathrm{um}} \frac{e^2 z_{ij}^2 \omega}{nc\epsilon_o}(N_i - N_j) \times \frac{\Gamma_{ij}/2}{(E_j - E_i - \hbar\omega)^2 + (\Gamma_{ij}/2)^2}, \tag{1}$$

where $n = \sqrt{\epsilon_\infty}$, "um" is the upper miniband, "lm" is the lower miniband, ω is the radian frequency, n is the refractive index, c is the velocity of light, e is the charge of an electron, $\hbar$ is the Planck's constant, E_j is the energy value of the upper level, E_i is the energy value of the lower level, N_i and N_j are the electron densities of subbands i and j, z_{ij} is the dipole matrix element between states *i* and *j*, and Γ_{ij} is the linewidth of absorption. The full width at half maximum (FWHM) of Γ_{ij} has been assumed to be 5% of the transition energy [2].

The absorption spectrum of the designed TPV structure is shown in Fig. 2 along with the blackbody radiation spectrum at 1500 K. The absorption spectrum has two peaks at ~0.36 eV and ~0.42 eV that cover a broad region of blackbody spectrum around the peak at 1500 K. The FWHM of the absorption spectrum is 95 meV which is 20% of the FWHM of the blackbody radiation spectrum at 1500 K and much greater than the FWHM of the similar TPV structures in Ref. [1].

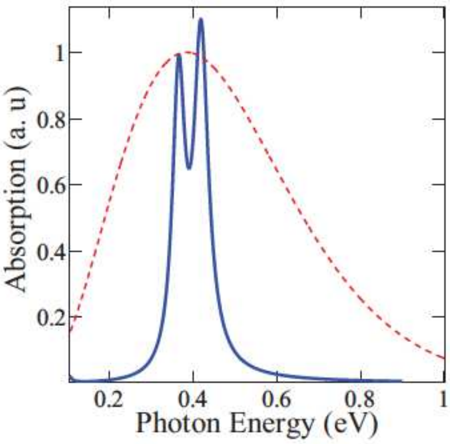

Fig. 2. Absorption spectrum of the designed TPV structure (solid line) and the blackbody radiation spectrum at 1500 K (dashed line).

IV. CURRENT-VOLTAGE RELATION

To calculate the V_{oc} due to the photo-excited carriers in the designed structure, we take an isolated period of the structure. The number of photo-excited carriers is calculated for an incident steady-state blackbody radiation at 1500 K. The electron-photon scattering rate is calculated by Fermi's golden rule [6], [7]

$$O_{ij} = \frac{2\pi}{\hbar}\left(\frac{eE_o}{m\omega}\right)^2 (<j|\vec{e}.\vec{p}|i>)^2 \frac{\Gamma/2}{(E_j - E_i - \hbar\omega)^2 + (\Gamma/2)^2}, \tag{2}$$

where m is the mass of an electron, ω is the frequency of the incident light, E_o is the electric field of the incident light, Γ is the linewidth of absorption, and i, j are the wavefunctions. The rate of relaxation of the excited electrons by emitting LO phonons is concurrently calculated. The electron-LO phonon scattering rate is given by [6]

$$W_{ul} = \frac{2\pi}{\hbar}|\langle l, k_l|H'_{\mathrm{e-ph}}|u, k_u\rangle|\partial(E_l(k_l) - E_u(k_u) \pm \hbar\omega_{\mathrm{LO}}), \tag{3}$$

where $H'_{\mathrm{e-ph}}$ is the electron-LO phonon interaction hamiltonian, k_u and k_l are the wave numbers of the upper and lower energy level, and $\hbar\omega_{\mathrm{LO}}$ is the LO phonon energy. Since the electrons are redistributed in space, Poisson's equation is solved to calculate the change in internal electric field. The internal electric field created due to the redistribution of carriers is added to the conduction band energy profile and then Schrödinger equation is solved to calculate the new wavefunctions and energy levels. Iterative solution of coupled Schrödinger and Poisson's equations in conjunction with the rate equations that include the electron excitation due to incident photons and relaxation of excited electrons due to LO phonon emission results electron density build-up in one side than that in the other side. Then from the difference of ground state energies of two neighboring stages, we find the V_{oc}. We can express the equation as

$$V_{\mathrm{oc}} = E_{1,p} - E_{1,(p-1)}, \tag{4}$$

where p is period number. In Fig. 1, the dashed line shows a change in the conduction band profile due to the accumulation of photo-excited carriers to the right side of the structure. In calculating *J*-*V* relation, a periodic boundary condition is assumed. So, input current to the structure is equal to the current leaving the structure.

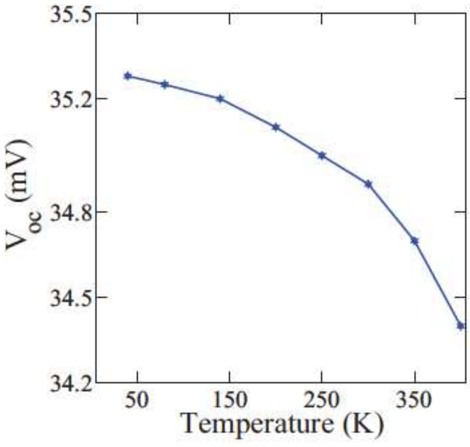

Fig. 3. The photo-generated open-circuit voltage (V_{oc}) of the designed TPV structure against temperature.

The V_{oc} of one stage of the structure is calculated as 35 mV at room temperature. The V_{oc} of the overall structure will be multiplied by the number of stages in the structure. In Fig. 3, we show V_{oc} against temperature. We note that V_{oc} decreases as the temperature increases. The J-V characteristics is shown in Fig. 4, which shows that the open-circuit voltage is approximately 35 mV per period and short-circuit current density of 2.94 $\mathrm{kA/cm^2}$ from this structure. It is also seen that the J-V relation does not exactly follow the well known exponential form of classical diode equation model as shown in [1]. Hence, a quantum mechanical model is necessary for characterization of such quantum cascade structures.

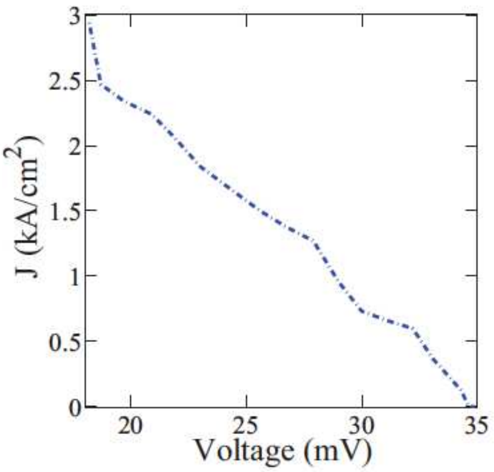

Fig. 4. Current-voltage (J-V) relation of the designed TPV structure using quantum mechanical model.

V. CONCLUSION

In conclusion, we designed a quantum cascade thermo photovoltaic structure using GaN/AlGaN material system. The designed structure absorbs over a broad range around ~0.4 eV of blackbody radiation at 1500 K. We developed a fully quantum mechanical model to calculate the open-circuit voltage and the current-voltage relation of the designed quantum cascade structure. The current-voltage relation of the thermo photovoltaic quantum cascade structure found using the developed model is different from that found using a semi-classical model.

ACKNOWLEDGEMENTS

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REFERENCES

[1] J. Yin and R. Paiella, "Multiple-junction quantum cascade photodetectors for thermophotovoltaic energy conversion," Opt. Express **18**, 1618–1629 (2010).
[2] M. Ahmed, A. K. M. D. Hossain, and M. A. Talukder, "Quantum cascade structures for efficient thermo-photovoltaic energy conversion," Photonics Global Conference (PGC 2012), Singapore (2012).
[3] J. Yin and R. Paiella, "Limiting performance analysis of cascaded interband/intersubband thermophotovoltaic devices," Appl. Phys. Lett. **98**, 041103–1—041103–3 (2011)
[4] H. Zhao, R. A. Arif, Y. K. Ee, and N. Tansu, "Self-Consistent Analysis of Strain-Compensated InGaN-AlGaN Quantum Wells for Lasers and Light Emitting Diodes," IEEE Journal of Quantum Electronics **45**, 66–78 (2009).
[5] S. L. Chuang and C. S. Chang, "A Band-structure model of strained quantum well wurtzite semiconductors," Semicond. Sci. Technol. **12**, 252-263 (1997).
[6] P. Harrison, *Quantum Wells, Wires and Dots* (Wiley, 2006).
[7] H. C. Liu, F. Capasso, *Intersubband Transitions in Quantum Wells: Physics and Device Applications II* (Academic Press, 2000).