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Heterostructured cathode with graded bandgap window-layer for photon-enhanced thermionic emission solar energy converters

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ABSTRACT

A heterostructured cathode having a graded bandgap window-layer is proposed in this study to improve the performance of photon-enhanced thermionic emission (PETE) solar energy converters. A model based on a one-dimensional steady-state equation is developed to analyze the characteristics of the proposed device. This model is used to calculate the conversion efficiency of a PETE device with an $\text{Al}_x\text{Ga}_{1-x}\text{As/GaAs}$ cathode. The built-in electric field induced by the bandgap gradation in the windowlayer is shown to improve the efficiency because of the reduction of contact surface recombination losses and efficient collection of photogenerated electrons. This field is unaffected by temperature variation, and the improvement of efficiency is sustained at elevated temperatures. The effect of window-layer parameters and cathode thickness on efficiency is discussed. We also show that the efficiency maximizes at lower temperatures for cathodes with lower electron affinities. Moreover an optimal value exists for anode work function at a given anode temperature, thus providing guidance for the optimum design of barrier conditions for both cathode and anode.

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1. Introduction

Photovoltaic (PV) solar cells and solar thermal converters are two conventional technologies used in solar energy conversion. Photovoltaic solar cells utilize the large per photon energy of a fraction of the solar spectrum. On the other hand, solar thermal converters utilize the energy of the entire solar spectrum; however, their conversion efficiency is inherently low [\[1\].](#page--1-0) Hybrid systems that combine PV solar cells and solar thermal converters have been proposed to combine the advantages of these technologies and are predicted to have high efficiency [\[2\]](#page--1-0). However, they fail in practice because conventional PV cells cease to operate at high temperatures [\[3\]](#page--1-0) whereas solar thermal converters lose efficiency at low temperatures.

Photon-enhanced thermionic emission (PETE) is a novel concept in solar energy conversion that utilizes both photon and thermal energy of incident solar radiation [\[1\]](#page--1-0). The proposed PETE device consists of a semiconductor cathode and an anode separated by a vacuum gap. The cathode is illuminated and heated by incident solar radiation. Electrons are excited by photons above the bandgap, thus increasing the conduction band population of the cathode. The photogenerated electrons rapidly thermalize within the conduction band, and those with energies greater than the electron affinity of the cathode are emitted into vacuum and collected by the anode. The theoretical conversion efficiency of a PETE device is predicted to be over 40% for an incident solar radiation concentration of 1000 at operating temperatures above 200 \degree C. PETE devices can harvest solar energy at elevated temperatures, and they can be used with heat engines in tandem to convert waste heat, thus increasing the total conversion efficiency to over 50%.

In recent years extensive effort has been made to analyze the characteristics of PETE devices, and different models and structures have been proposed $[4-7]$ $[4-7]$. Varpula and Prunnila $[8]$ presented a one-dimensional (1-D) model that included bulk and surface recombination, spatial distribution, and diffusion of photogenerated carriers. The results showed that surface recombination can drastically reduce conversion efficiency. Another analytical model based on 1-D steady-state diffusion treatment has been proposed for both photocathodes and PETE cathodes [\[9\]](#page--1-0). Recombination at the emissive surface is shown to be critical to internal quantum yield of PETE devices, and surface passivation is proposed as a means to achieve high PETE efficiencies. Recently, a heterostructure cathode with low interface recombination has been proposed for PETE applications [\[10\]](#page--1-0). The cathode consists of a GaAs absorber layer and a nanoscale AlGaAs emitter layer, which passivates the emissive surface. The measurements show that the quantum efficiency of the heterostructure cathode is significantly improved.

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A cathode with a homojunction back surface field (BSF) layer was proposed to reduce surface recombination losses at the contact surface and improve device performance [\[11\].](#page--1-0) The BSF layer is implemented by varying cathode doping near the cathode contact, and a barrier is thus established to repel electrons from the contact surface. However, the barrier height is limited by the bandgap and the doping level of the cathode material. The barrier formed owing to the doping variation decreases with increasing temperature, thus reducing device efficiency at elevated temperatures [\[11\].](#page--1-0)

For a photocathode with structure similar to that of a PETE cathode, the contact surface recombination losses are reduced by introducing a window-layer material with a greater bandgap between the cathode and the contact [\[12,13\].](#page--1-0) The heterostructured cathode was also proposed for PETE applications in Ref. [\[11\]](#page--1-0) to solve the problem of homojunction deterioration. The windowlayer can serve as a passivation layer that reduces defects at the back interface [\[14\]](#page--1-0). Furthermore, the greater bandgap of the window-layer presents a potential barrier to photogenerated electrons in the absorber that reflects the electrons away from the contact surface [\[15\]](#page--1-0). This barrier formed by the conductive band discontinuity at the heterojunction interface functions at elevated temperatures. However, in solar energy conversion, photons with energy greater than the bandgap of the windowlayer material will be absorbed in a region adjacent to the contact surface. These electrons will be lost, owing to surface recombination, instead of being collected and utilized as electric power. Therefore a fraction of the solar spectrum is unused, and thus the conversion efficiency is reduced.

The contact surface recombination can also be reduced by introducing a built-in electric field induced by the bandgap gradation in the window-layer. This field not only repels electrons from the contact surface at elevated temperatures but also efficiently collects short wavelength photons. Graded bandgap structures have been previously used in $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{Ga}$ As and CdHgTe solar cells $[16-18]$ $[16-18]$ and $Al_xGa_{1-x}As/GaAs$ photocathodes [\[19\]](#page--1-0). In this study, we will investigate the prospect of using a heterostructured cathode with graded bandgap window-layer to improve the performance of PETE devices.

2. Structure and principle

In this study, the cathode with the graded bandgap windowlayer is implemented using an $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{Ga}$ As heterostructure, whose schematic band diagram is shown in Fig. 1. The band bendings near the surface and interface are neglected. S_1 , S_2 , and S₃ are recombination velocities of contact surface, heterojunction interface, and emissive surface, respectively. d_1 is the windowlayer thickness, d_2 is the absorber thickness, E_F is the Femi level, J_{in}

Fig. 1. Schematic band diagram of heterostructured cathode with graded bandgap window-layer.

is the injected current from window-layer to absorber, and E_g is the bandgap of absorber. E_{g_1} and E_{g_2} are the bandgaps of $\text{Al}_{x}\text{Ga}_{1-x}$ As at the contact surface and heterojunction interface, respectively. The heterostructured cathode consists of a graded bandgap $\text{Al}_x\text{Ga}_{1-x}$ As window-layer and a GaAs absorber with a uniform bandgap and doping level. The bandgap gradation is achieved by varying the proportion of Al from 0.3 to 0.1 in the $\text{Al}_{x}\text{Ga}_{1-x}$ As layer. As shown in Fig. 1 only the conduction band minimum is assumed to be influenced by the gradient in Al concentration, and the valence band maximum is assumed to remain fixed. This assumption is valid because for $\text{Al}_x\text{Ga}_{1-x}\text{As}$, the affinity of electrons decreases by almost the same amount as the bandgap increase with increasing x [\[20\].](#page--1-0) The doping level of the window-layer varies within the range of 1.3305 \times 10¹⁹–1.1636 \times 10^{19} cm $^{-3}$ from the contact surface to the interface, whereas the doping level of the absorber is 1×10^{19} cm⁻³. The built-in electric field induced by the compositional grade is given by

$$
E = \frac{E_{g_2} - E_{g_1}}{d_1 q},\tag{1}
$$

where q is the electron charge.

The solar radiation is incident perpendicular to the cathode contact surface. In the $E_{g_2} > h \nu \geq E_g$ spectral region, photons are absorbed deep inside the cathode in the absorber because of the window effect. The electrons that are generated by the photons with energy $h\nu>E_{g_2}$ in the window-layer are accelerated by the electric field toward the heterojunction interface. Subsequently, the electrons that reach the interface are injected into the absorber and contribute to the conduction band population of the absorber. The built-in electric field produced by the bandgap gradation prevents the contact surface recombination losses, and the electrons are efficiently collected, thus leading to enhanced conversion efficiency.

3. One-dimensional analysis

In this analysis, space-charge effects and temperature gradients in cathode and anode are not taken into account. We assume that the voltage difference is mainly across the vacuum gap. The applied electron field inside the cathode is zero. The photogenerated carriers are assumed to support the local charge neutrality approximation. The cathodes are assumed to operate under low injection conditions, wherein the excess electron concentration is smaller than the equilibrium concentration of holes in both the window-layer and the absorber. In the steady state, the continuity equation for excess electrons in the graded bandgap window-layer is

$$
\frac{d^2 n_1}{dx^2} + \frac{\mu_n E}{D_{n1}} \frac{dn_1}{dx} - \frac{n_1}{L_{n1}^2} + \frac{G_1(x)}{D_{n1}} = 0,
$$
\n(2)

where n_1 is the excess electrons concentration, and D_{n_1} is the electron diffusion coefficient. In addition, L_{n_1} is the electron diffusion length, and μ_n and $G_1(x)$ denote electron mobility and the photon generation function of the electrons, respectively.

Under low injection level, the electron diffusion length is assumed to be independent of the excess electron concentration and the general solution of Eq. (2) exists. The general solution of the continuity equation can be given as $[18]$

$$
n_1(x) = C_1 \exp(\Lambda_1 x) + C_2 \exp(\Lambda_2 x) + \frac{1}{\Lambda_1 - \Lambda_2} [\exp(\Lambda_1 x) F_1(x) + \exp(\Lambda_2 x) F_2(x)],
$$
\n(3)

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