Open-Circuit Voltage of an Illuminated Nonideal Heterojunction

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Abstract—The possibility of using the model of tunneling-recombination transport for calculating the photovoltage of an illuminated nonideal heterojunction is demonstrated. The technique of photoexcitation with light of varying spectral composition is used, and the difference in the behavior of the dependence of the photovoltage on the illumination is explained. The heterojunction photovoltage is calculated taking into account the predominance of the tunneling-recombination transport mechanism in the barrier region and modification of the shape of the potential barrier during illumination. It is shown that the dependences calculated at various illumination levels agree with those obtained experimentally.

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1. INTRODUCTION

In [1] we proposed the method of using the Mott model [2] (tunnel–hopping conductivity developed for noncrystalline materials) for describing the conductivity of inhomogeneous structures, for example, that in the space-charge region (SCR) of a nonideal heterojunction. How to take into account the effect of processes occurring at the heteroboundary of such structures for calculation of the current flow and the photovoltage characteristic is also shown. At the same time, it was shown in [3, 4] how the illumination of a nonideal heterojunction can modify the SCR width in the heterojunction and the potential-barrier shape, thus affecting its conductivity [5]. All of this must be taken into account when determining the photovoltage of an illuminated nonideal heterojunction.

2. DETERMINATION OF THE PHOTOVOLTAGE OF AN ILLUMINATED NONIDEAL HETEROJUNCTION

For definiteness’ sake, we further consider the CdS–Cu2S heterojunction, which represents a sharply asymmetric structure in which almost the entire SCR is localized in high-resistivity CdS. According to [6], the expression for the $I–V$ characteristic of the illuminated heterojunction has the form

$$ j = n_e \exp\left(\frac{-\varphi_0}{kT}\right) e^{s_\delta} \exp\left(\frac{eU}{kT} - 1\right) \cdot \frac{e \varphi_0 L \gamma \eta}{\varphi_0 + s_\delta} - \frac{e \varphi_0 L \gamma \eta}{\varphi_0 + s_\delta}. \quad (1) $$

Here, $n_e$ is the concentration of majority carriers in the quasineutral region of CdS, $\varphi_0$ is the barrier height, $s_\delta$ is the surface-recombination rate, $\varphi_\delta$ is the drift rate at the heteroboundary, $L$ is the incident-energy density, $\gamma$ is the collection coefficient in Cu2S (disregarding the losses at the heteroboundary), and $\eta$ is the quantum yield. It should be kept in mind that it was only the thermal-diffusion mechanism of current transfer that was considered in [7]; i.e., tunnel-hopping mechanisms were disregarded in Eq. (1).

From formula (1), it is easy to obtain the expression for the open-circuit voltage $U_{oc}$ of the illuminated heterophotocell assuming that $j = 0$:

$$ \frac{\varphi_\delta}{\varphi_\delta + s_\delta} L \gamma \eta = \left(\frac{\varphi_\delta}{\varphi_\delta + s_\delta} L \gamma \eta + e \varphi_\delta n_0\right) \times \frac{\varphi_0 e^{s_\delta}}{\varphi_\delta + s_\delta} \left(e^{\varphi_0/kT} - 1\right). \quad (2) $$

Here, the left-hand side determines the flux of electrons photogenerated in the Cu2S region through the interface, and the right-hand side, the reverse thermal-diffusion current. The calculation shows that the following inequality is always fulfilled with increasing stimulating-light intensity up to solar light intensity for the CdS–Cu2S heterojunction:

$$ \frac{\varphi_\delta}{\varphi_\delta + s_\delta} L \gamma \eta \ll e \varphi_\delta n_0. \quad (3) $$

Taking into account (3), after simple transformations, it is easy to obtain an obvious expression for determining $U_{oc}$ from Eq. (2). Taking into account that
In the CdS quasineutral region and designating \( L \gamma \eta = j_0 \), we obtain

\[
U_{oc} = \varphi_0 + kT \ln \left( \frac{j_0}{e \delta \eta N_D} + e^{\frac{U_{oc}}{kT}} \right). \tag{4}
\]

From (4), it can be seen that the open-circuit photovoltage of the illuminated sample is independent of the parameter \( \varphi_0 \) (hence, it is independent of the shape of the potential barrier), and is determined only by the generation rate of carriers in Cu\(_2\)S and their recombination rate at the heteroboundary.

The value of \( U_{oc} \) is determined from the condition of equality of two carrier fluxes, i.e., from Cu\(_2\)S to CdS and the reverse flux from CdS to Cu\(_2\)S, caused by various mechanisms of carrier transport through the barrier. The mechanisms can be both thermally activated and tunneling in character. Introducing the tunneling-recombination currents \( (j_T) \) flowing through the potential barrier in the model and taking into account inequality (3), we transform (2) to a more general form:

\[
\frac{V_0}{s_0} = L \gamma \eta = e \frac{\varphi_0}{s_0} \frac{kT}{e} \left( \frac{U_{oc}}{kT} - 1 \right) + j_T. \tag{5}
\]

Now the right-hand side determines both the reverse thermal-diffusion and tunneling-recombination currents. To calculate \( j_T \) caused by the motion of carriers along localized states and their recombination at the interface, it is necessary to specify the barrier height \( \varphi_0 - U_{oc} \) and its width \( \omega \), and also the dependence \( \varphi(x) \), which, according to [3, 4], under illumination conditions can dramatically differ from quadratic law, which greatly affects the value of \( \varphi_0 \) determining the left-hand side of (5).

Under conditions of the excitation of wide-gap CdS in which the barrier is localized, it is possible to determine these parameters unambiguously, specifying the values of the dark capacitance \( C_0 \) and junction photocapacitance \( C_L \). When carrying out the experiment and for calculations, it is convenient to use the dependences \( V_0(C_D, U_{oc}), U_{oc}(C_L), j_T(C_L, U_{oc}) \). If we assume that the cell is irradiated with only long-wavelength light, then the specified parameters are only determined the decrease in the barrier height to a value of \( \varphi_0 - U_{oc} \) for its arbitrary intensities and a certain decrease in its width related to it. The estimated calculations show that, for \( U_{oc} < 0.7 \text{ V} \) (valid to solar-light illumination), the tunneling-recombination current \( j_T \) exceeds the thermal-diffusion component by several orders of magnitude.

This means that, for low stimulating-light intensities, (5) for determining \( U_{oc} \) in a nonideal heterojunction is simplified to the form

\[
L \gamma \eta \frac{V_0(U, C_L)}{V_0(U, C_\varphi)} = j_T(U, C_\varphi). \tag{6}
\]

As was noted above, the tunneling currents and recombination at the interface of the nonideal heterojunction significantly affect its photoelectric properties. The problem of photovoltage losses is relatively complex because here it is necessary to take into account the decrease in the free-carrier flux, which intersects the heteroboundary due to recombination, instead of just the flux itself, and also efficient shunting of the barrier by the tunneling currents.

### 3. EXPERIMENTAL RESULTS

In Fig. 1, we show the experimentally obtained dependences of the open-circuit voltage for the illuminated CdS–Cu\(_2\)S photocells on the photocapacitance \( C_L \) depending on the intensity of stimulating white light.

![Fig. 1. Experimental dependences of the open-circuit voltage of illuminated CdS–Cu\(_2\)S photocells on the value of the photocapacitance \( C_L \) depending on the intensity of stimulating white light.](image)