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Studies on n-CdTe/p-$CuInSe_2$ heterojunctions

J. J. B. Prasad, D. Krishna Rao, and J. Sobhanadri
Department of Physics, Indian Institute of Technology, Madras-600 036, India

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n-CdTe/p-$CuInSe_2$ heterojunctions were fabricated by flash evaporating p-$CuInSe_2$ on indium-doped CdTe single crystals. I-V characteristics and the photospectral response of the heterojunctions were studied. On illumination appreciable change in the I-V characteristics and photovoltaic effects were observered. A theoretical energy-band diagram for the heterojunction was constructed, and the theoretical and experimental barrier potentials were compared.

I. INTRODUCTION

The important application of heterojunctions has been identified in the photonic devices including photodetectors, solar cells, light-emitting diodes, and semiconductor lasers. The wide range of these technological applications is discussed in detail by Milnes and Feucht,[1] Sharma and Purohit,[2] Casey and Panish,[3] and Sze.[4] For photodetector and solar cell applications, semiconductors other than silicon which have an energy gap between 1.1–1.6 eV, are especially preferred[5] to obtain optimum efficiencies. During the last decade several studies on heterostructures using CdS[6–8] have been made for photovoltaic applications. CdS-$CuInSe_2$ is the widely studied heterostructure for solar cell applications because of its good lattice match and the absence of any interfacial spike in the conduction band.[9–11] Heterostructures based on CdTe have also been studied in recent years because of CdTe's importance for a wide range of applications including photovoltaics and radiation detectors.[12,13] The InSb-CdTe heterostructure system is well studied[14,15] in this group because of the perfect lattice match between these materials. $CuInSe_2$ is a direct band-gap semiconductor (1.04 eV) belonging to the I-III-VI_2 group of semiconductors with chalcopyrite structure. Several studies have been made on this material from fundamental as well as application points of view. Several heterostructures using this material in combination with GaSe,[16] InSe,[17] CdS,[10] etc., have been studied from the technological point of view. We have fabricated CdTe/$CuInSe_2$ heterostructures by depositing p-type $CuInSe_2$ thin films on n-type CdTe single crystals. Even though the lattice mismatch between CdTe and $CuInSe_2$ is high, we have observed good photovoltaic effects in the system. In this paper we report the results obtained on the I-V characteristics and photoresponse studies on CdTe/$CuInSe_2$ heterojunctions. A theoretical energy-band diagram for this heterostructure is constructed, and the results of I-V characteristics and photoresponse studies are discussed.

II. EXPERIMENTAL DETAILS

n-type CdTe single crystals doped with indium, grown by the Bridgman–Stockberger method, were used in the present study. The resistivity of the as-grown crystals was found to be 0.15 Ω cm and the carrier concentration (N_d) was estimated as $3.8\times10^{16}/cm^3$. From photoconductivity experiments the band gap of the material was found to be 1.44 eV. The as-grown crystals were sliced, lapped, and finally etched with a bromine/methonol solution. Samples of size $2\times2\times1$ mm were used in the present study. Copper indium selenide bulk material was prepared by vacuum fusing the high-purity constituent elements at 1150 °C. The detailed growth process and transport properties are mentioned in detail elsewhere.[18] The composition of the charge was tested using x-ray diffraction and electron probe microanalysis techniques, and the material was found to be in the required single phase. $CuInSe_2$ films of thickness 0.5 μm were grown on CdTe single crystals and glass substrates by evaporating the $CuInSe_2$ charge at 10^{-6} Torr vacuum using a simple flash evaporation technique developed in the laboratory.[19] The substrates were kept at 250 °C and the film deposition rate was about 100 Å/s. Samples obtained on glass substrates are used for characterizing the $CuInSe_2$ films. The films were found to be p type in nature and to have resistivity of the order 8 Ω cm. The carrier concentration (N_a) in these films was found to be $2.6\times10^{16}/cm^3$ and mobility = 30 cm^2/V s. A semitransparent gold film of thickness 450 Å was vacuum deposited over the $CuInSe_2$ film of the grown CdTe/$CuInSe_2$ heterostructure using thermal evaporation. The back contacts on n-CdTe single crystals were obtained by soldering indium. The ohmic contact nature for In/CdTe and Au/$CuInSe_2$ was tested separately prior to the factrication of the heterostructures.

III. RESULTS

I-V characteristics of CdTe/$CuInSe_2$ heterojunctions (HJ) in dark and illuminated conditions at 300 K are shown in Fig. 1. Illumination has been done using a tungsten lamp on $CuInSe_2$ side through the transparent gold contact. In dark conditions the heterostructure had good rectification properties and on illumination (80 m W/cm^2) considerable change was observed in the reverse bias (CdTe positive). In forward characteristics no appreciable change has been observed on illumination. Since the dark I-V plots were similar to the diode characteristics, the current-voltage relation in heterojunction can be written as $I \propto \exp(qV/nkT)$, where q is electronic charge, n is the ideality factor, and kT has the usual meaning. The semilog plot of forward I-V characteristics of the heterojunction is shown in Fig. 2. The n values

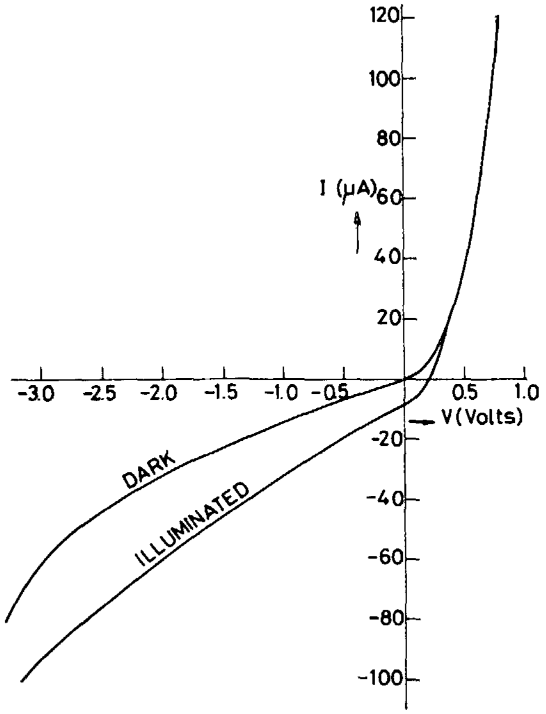

FIG. 1. A typical I-V characteristic of $CdTe/CuInSe_2$ heterostructure in dark and illuminated conditions at 300 K.

were found to vary from 1.3 to 4.6 in the voltage range 0–0.85 V. The reverse saturation current was obtained by extrapolating the forward I-V characteristics at low voltages where n values are of the order of 1 and the value was found to be 1×10^{-7} A.

Photo response studies were also made on these HJ devices using a tungsten lamp as a light source. When the junction was illuminated with intensity 100 mW/cm^2, an open circuit voltage of 400 mV and short-circuit current 2 mA/cm^2 were obtained. The photospectral response was studied using the Carl–Zeiss monochromator in the spectral region 400–1100 nm. The normalized photoresponse corrected to the lamp intensity is shown in Fig. 3. At 765 nm a prominent peak was observed in the experimental curve. The square root of the response per each photon versus photon energy was plotted (Fowler plot) in Fig. 4. By extrapolating the straight line obtained, the barrier potential of the system was found to be 1.26 eV.

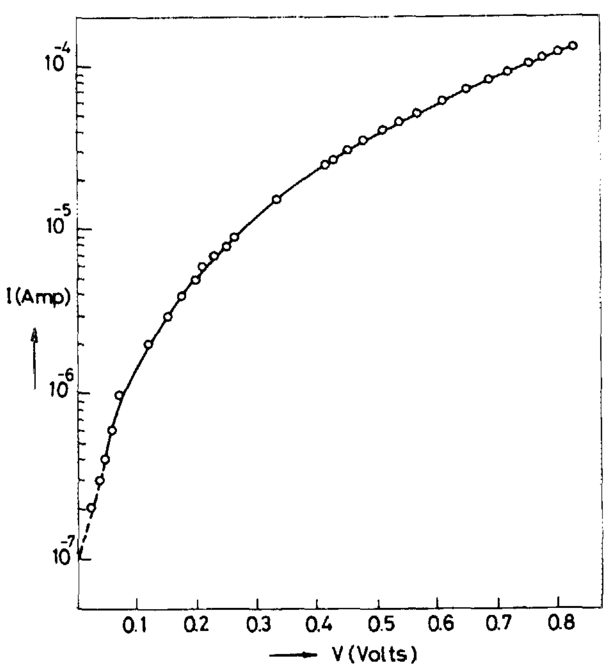

FIG. 2. Semilogarithmic plot I-V characteristic of $CdTe/CuInSe_2$ heterostructure.

Based on the Anderson[20] model for the ideal heterojunction a theoretical energy-band diagram for n-CdTe/p-$CuInSe_2$ heterojunction was constructed as shown in Fig. 5. The values of various parameters used in constructing the band diagram are given in Table I. Since the work function of CdTe (4.40 eV) was less compared to that of $CuInSe_2$ (5.39 eV), the band bending at the junction will be as shown in Fig. 5. Hence, the theoretical barrier height (V_D) of the system was found to be 0.99 eV. The discontinuities in the conduction band (ΔE_c) and in the valence band (ΔE_v) were found to be 0.22 and 0.18 eV, respectively. The barrier heights in the n-type (V_{Dn}) and p-type (V_{Dp}) semiconductors were also obtained using the equation

$$V_D = V_{Dn} + V_{Dp}, \tag{1}$$

$$\frac{V_{Dn}}{V_{Dp}} = \frac{N_a \epsilon_p}{N_d \epsilon_n}, \tag{2}$$

where ϵ_p and ϵ_n are the dielectric constants of p- and n-type semiconductors, respectively. The values of V_{Dn} and V_{Dp} were found to be 0.38 and 0.61 eV, respectively. From the above heterostructure model one can observe that the potential barrier for electrons in the conduction band is low compared to that for holes in the valence band. Hence, when the junction is forward biased ($CuInSe_2$ positive), most of the conduction is dominated by the electrons moving from CdTe to $CuInSe_2$.

Using the above energy-band diagram, the value of the barrier potential was also derived from the I-V characteristics by following the thermionic emission and diffusion model as

$$I = I_0 \exp(qV/kT), \tag{3}$$

where

$$I_0 = qaN_d \frac{D_n}{L_n} \exp - \left(\frac{V_D - \Delta E_c}{kT}\right). \tag{4}$$

In Eq. (4) a is the area of the junction, D_n is the diffusion coefficient of electrons in p-type $CuInSe_2$ (11.2 $cm^{-2}\,s^{-1}$), and L_n is the diffusion length of electrons in $CuInSe_2$ (2.51 μm), respectively.[21] Using Eq. (3), the barrier height V_D was calculated as 0.64 eV. The results of the above findings are discussed in the following section.

IV. DISCUSSION

From Fig. 1 one can observe that in the forward and reverse bias conditions current initially increases slowly with

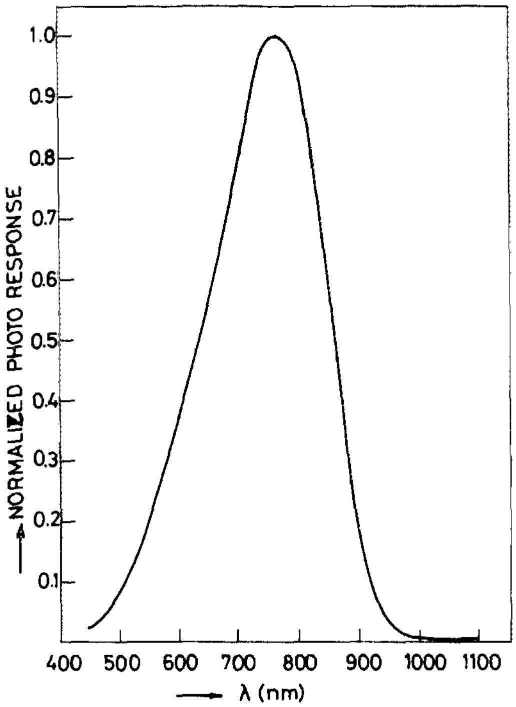

FIG. 3. Photospectral response CdTe/$CuInSe_2$ heterostructure.

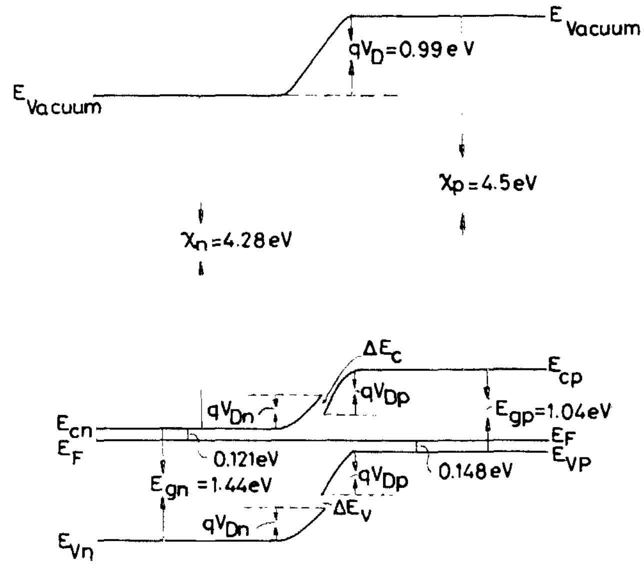

FIG. 5. Theoretical energy-band diagram of CdTe/$CuInSe_2$ heterostructure.

the voltage ($I \propto V$) and that after a certain voltage it follows a relation $I \propto V^m$, where m is nearly equal to 2 in the present case. The values of the transition voltages in the forward and reverse conditions were found to be 0.35 and 0.8 V, respectively. In the present investigation the value of n was found to increase from 1.3 to 4.6 in the experimental voltage range.

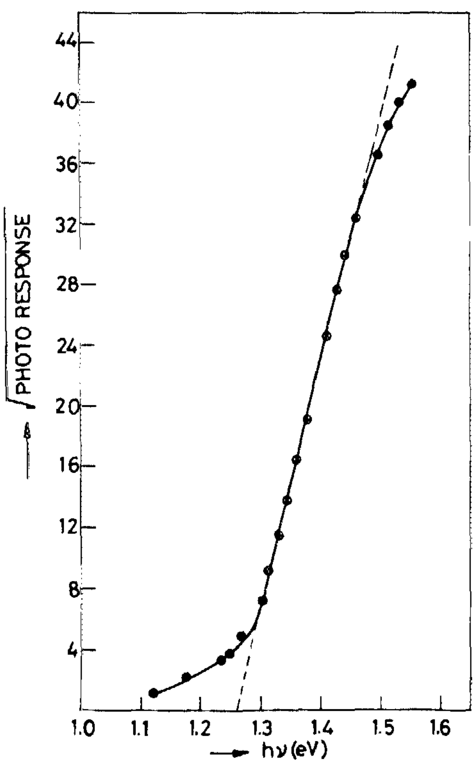

FIG. 4. Fowler plot of CdTe/$CuInSe_2$ heterostructure.

This indicates that at lower voltages the transport of carriers across the barrier was by diffusion process. But at higher voltages the increase in n values indicates that most of the carriers were recombined at the junction region. Hence, as the voltage increases, the current is limited by the carrier recombination. This could be due to the lattice mismatch of the CdTe/$CuInSe_2$ system, which may give rise to a large number of interface states. From the theoretical energy-band diagram it is clear that electrons contribute most of the current in HJ. The value of the barrier height obtained from *I-V* characteristics using the above model was found to be low compared to the theoretical value.

When the junction was illuminated through the gold contact, excess carriers were generated in the depletion region at the junction; these carriers were drifted across the potential barrier of the HJ, giving rise to a short-circuit current of 2 mA/cm^2. In the reverse bias condition upon illumination the excess carrier current was more; hence, the dark reverse characteristics deteriorated. From Fig. 3, the photoresponse of the CdTe/$CuInSe_2$ heterostructure shows a long wavelength cutoff around 850 nm. This region approximately corresponds to the band gap of CdTe. No appreciable photoresponse was observed near the wavelength region corresponding to the band gap of $CuInSe_2$. However, at the longer wavelength side, the photoresponse was found to start near the band-gap region of $CuInSe_2$. The absence of a peak around 1 eV in the photoresponse curve may be due to the recombination of photocarriers at the interface of the CdTe/$CuInSe_2$ heterojunction. To demonstrate clearly the role of $CuInSe_2$ in the photovoltaic properties of the HJ's, we have fabricated CdTe/Au Schottky devices and studied the effect of illumination on the *I-V* characteristics. Although good rectification properties were observed in these devices, no illumination effect was observed on the *I-V* characteristics. Also, practically no photovoltaic effects were observed in these devices. Therefore, the observed photovoltaic effects in the CdTe/$CuInSe_2$ HJ devices clearly indicate the existence of a *p-n* junction at the interface of CdTe and $CuInSe_2$,

TABLE I. Values of various parameters of CdTe and $CuInSe_2$ at 300 K.

Material	Band gap (eV)	Electron affinity (eV)	Carrier concentration (cm^{-3})	Fermi-level position (eV)	Dielectric constant	Lattice constants (Å)
n-CdTe	E_{gn}:1.44	χ_n:4.28	N_d:3.8×10^{16}	From the conduction band $E_{cn} - E_F$:0.121	ϵ_n:10.2	a: 6.48
p-$CuInSe_2$	E_{gp}:1.04	χ_p:4.50	N_a:2.6×10^{16}	From valence band $E_F - E_{vp}$:0.148	ϵ_p: 9.3	a: 5.85 c:11.75

which indirectly demonstrates the effect of $CuInSe_2$.

The values of the barrier potential obtained from photoresponse and I-V characteristics did not match in the present case. The value obtained from the photoresponse studies (1.26 eV) was higher than the theroetically predicted value (0.99 eV), and it is about $2\times$ the value obtained from I-V measurements (0.64 eV). The value obtained from I-V characteristics using the thermionic emission and diffusion model was found to be reasonable because it is close to the value of the open-circuit voltage (0.40 V) observed and also close to the knee voltage (0.43 V) of the forward I-V characteristics. The results of the present studies can be concluded as follows:

(1) Even though the lattice mismatch is high in CdTe/$CuInSe_2$ heterostructure, we have observed good rectification properties and appreciable illumination effects in the I-V characteristics and photovoltaic effects in this system.

(2) The value of the barrier potential obtained from I-V characteristics was found to be reasonable in CdTe/$CuInSe_2$ HJ since it is close to the value of the open-circuit voltage and the knee voltage observed in the forward I-V characteristics.

(3) Even though the effect of $CuInSe_2$ is not seen clearly in the photoresponse curve, the existence of a p-n junction at the interface of CdTe and $CuInSe_2$ has been verified on comparing the I-V characteristics (in illuminated conditions) of the CdTe/$CuInSe_2$ heterojunction and CdTe/Au structures.

[1]A. G. Milnes and D. L. Feucht, *Heterojunctions and Metal Semiconductor Junctions* (Academic, New York, 1972).
[2]B. L. Sharma and R. K. Purohit, *Semiconductor Heterojunctions* (Pergamon, London, 1974).
[3]H. C. Casey and M. B. Panish, *Heterostructure Lasers* (Academic, New York, 1978).
[4]S. M. Sze, *Physics of Semiconductor Devices* (Wiley, New Delhi, 1981).
[5]J. J. Loferski, J. Appl. Phys. **27**, 777 (1976).
[6]S. Wagner, J. L. Shay, K. J. Bachmann, and E. Buehler, Appl. Phys. Lett. **26**, 229 (1975).
[7]L. L. Kazmerski, F. R. White, M. S. Ayyagiri, Y. J. Juanig, and R. P. Patterson, J. Vac. Sci. Technol. **14**, 65 (1977).
[8]R. Hill, *Active and Passive Thin-Film Devices*, edited by T. J. Coutts (Academic, New York, 1978).
[9]J. L. Shay, S. Wagner, and H. M. Kasper, Appl. Phys. Lett. **27**, 89 (1975).
[10]L. L. Kazmerski, F. R. White, and G. K. Margan, Appl. Phys. Lett. **29**, 268 (1976).
[11]Y. Kokubun and M. Wada, Jpn. J. Appl. Phys. **16**, 879 (1977).
[12]J. Sarie, Shin-Ichi Yama Giwa, H. Matsunemi, and Tetsuro Tanaka, Solid State Electron. **24**, 845 (1981).
[13]P. Siffert, Nucl. Instrum. Methods **150**, 1 (1978).
[14]B. Rabin, C. Scharager, M. Hage-ali, P. Siffert, F. V. Wald, and R. O. Bell, Phys. Status Solidi **62**, 237 (1980).
[15]I. V. Varlamov, L. A. V'Yukov, A. M. Gulyev, L. P. Lazarenko, and A. N. Solyakov. Sov. Phys. Semicond. **14**, 1213 (1980).
[16]A. Sh. Abdinov, A. G. Kyazyn-Zade, V. K. Mamedov, and V. I. Tagirov, Sov. Phys. Semicond. **15**, 365 (1981).
[17]A. G. Kyazym-Zade, V. I. Tagirov, A. Sh. Abdinov, and V. K. Mamedov, Sov. Phys. Semicond. **16**, 222 (1982).
[18]D. Sridevi and K. V. Reddy (unpublished).
[19]D. Dridevi, J. J. B-Prasad, and K. V. Reddy, Bull. Mater. Sci. (in press).
[20]R. L. Anderson, Solid State Electron. **5**, 341 (1962).
[21]J. Piekoszeski, L. Castauer, J. J. Loferski, J. Bell, and W. Giriat, J. Appl. Phys. **51**, 5375 (1980).