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Photovoltaic effect in *p*–SiC/*p*–Si heterojunction

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The photovoltaic effect of isotype heterojunction with hole conductivity formed films of nanocrystalline *p*–21R–SiC, deposited on single-crystal substrate of *p*–Si, has been studied (heterojunction *p*–SiC/*p*–Si). The films were prepared by direct ion deposition. The features of the current-voltage and the photovoltaic characteristics of the heterostructure *p*–SiC/*p*–Si were explained by the effect of the potential barriers, caused by band offsets in the contact region, on the migration of charge carriers through the heterojunction.

Исследован фотовольтаический эффект в изотипном гетеропереходе с дырочной проводимостью, образованном пленками нанокристаллического p–21R–SiC, осажденными на монокристаллические подложки из p–Si (гетеропереход *p*–SiC/*p*–Si). Пленки получали методом прямого ионного осаждения. Особенности вольтамперных и фотоэлектрических характеристик гетероструктуры *p*–SiC/*p*–Si объяснены влиянием потенциальных барьеров, обусловленных разрывами зон в контактной области, на миграцию носителей заряда через гетеропереход.

1. Introduction

The main problems confronting solar power engineering comprise the increase of the conversion efficiency, reduction of the costs and rise of the radiation resistance of solar elements. Therefore, silicon carbide which possesses high radiation, thermal and chemical stability may turn out to be one of the materials suitable for this purpose. Up to now there has been reported creation of photoelectroconverters based on *p*–SiC/*n*–Si heterostructure [1–3]. Depending on the technology of the obtaining of the heterostructure and the crystalline structure of SiC, the efficiency of the photoelements ranged between 0.1 % for nanocrystalline SiC obtained by the method of plasmic chemical vapor deposition [1] and 14 % for nanocrystalline SiC obtained by hot-wire chemical vapor deposition [2]. It should be noted that the application of *n*-silicon in the studied heterostructures limits their use as photoconverters for radiation devices. As is known [4, 5], *n*-silicon is much more sensitive to the action of radiation than *p*-silicon. Therefore, the latter is nowadays used in the capacity of base layer while making silicon solar batteries meant for space experiments.

The anisotropic heterojunction *p*–SiC/*n*–Si studied in [1–3] have the value of the contact field of the depletion layer E_{intr} higher than the one of *p*–SiC/*n*–Si, *n*–SiC/*p*–Si and *p*–SiC/*p*–Si heterojunction. For the case of *p*–SiC/*n*–Si heterojunction the potential barriers created by bendings of the conduction and valence bands have the maximum height. The change of the type of conductivity in any of the heterostructure layers may lead to a considerable variation of E_{intr} value defined by the difference in the works functions $\Delta\varphi$. The change of the energy band pattern of the heterojunction will vary its photoelectrical characteristics and parameters. Therefore, it is significant to investigate photovoltaic effect in the isotype heterojunction SiC/Si. The goal of the present work was to obtain the heterostructure SiC/Si with hole-type conductivity and to study its photoelectrical properties. Up to now the possibility to use *p*–SiC/*p*–Si heterostructures in the capacity of photoelectroconverters has not been investigated.

2. Experimental

The heterostructure *p*–SiC/*p*–Si was formed by deposition of nanocrystalline silicon carbide (nc–SiC) films on a *p*-doped single-crystalline silicon substrate of KDB-4,5 type. The deposition was realized on a setup for direct ion deposition [6]. Carbon and silicon ion flows were generated using a vacuum arc plasma source with reaction bonding silicon carbide cathode. The average energy of carbon and silicon ions was ~120 eV. For the obtaining of silicon carbide films with hole-type conductivity there was used the ability of silicon carbide for self-doping. The type of conductivity depends on the method of SiC self-doping — by carbon or silicon ions [7]. The acceptor dopants at silicon carbide self-doping are silicon vacancies, i.e. excessive carbon atoms. Therefore, the ratio C:Si in *nc*–SiC films equal to 1.08 was provided at the excess of carbon. After the formation of SiC film the type of its conductivity was defined more exactly by measuring the value of thermo-emf.

In accordance with the earlier defined technological conditions [8] there were grown nc–SiC films of the rhombohedral polytype 21R. The choice of this polytype is caused by the fact that its forbidden band width exceeds that of the cubic polytype, and the growth temperatures are lower in comparison with the ones of the hexagonal polytypes [8]. The thickness of nc–21R–SiC films varied from 200 nm to 1000 nm, the average size of the nanocrystallites earlier determined by the methods of X-ray structure and electron microscopic analysis was 10–15 nm [8].

After creating metallic contacting layers on the surface of SiC there were realized photolithographic processes to obtain a pattern of the required configuration. Ohmic metal — nc–SiC contact was produced using a nickel layer with the thickness d_{Ni} = 0.1 μm by the method of magnetron deposition with subsequent vacuum annealing. Afterwards titanium (d_{Ti} = 300 Å) and gold (d_{Au} = 1000 Å) layers were applied by thermal deposition, and a layer of gold (d_{Au} = 1.5 μm) was deposited by galvanic method. Prior to the deposition processes the plates underwent chemical cleaning in organic solvents. The metals were pickled by means of solutions with a special composition. The quality of the contacting pattern was improved by two photolithographic processes performed onto the deposited nickel layers prior to annealing the contact, and onto the formed layers of titanium and gold. The area of the semitransparent metallic contact obtained on the surface of SiC was 2.4 mm^2. On the silicon substrate the metallic ohmic contact was formed on the whole of the substrate surface by magnetron deposition.

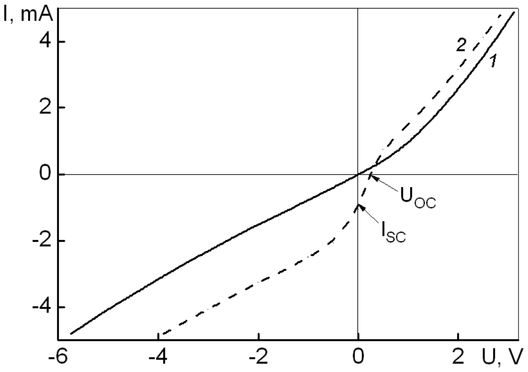

Fig. 1. *I–V* characteristics of *p*–21R–SiC/*p*–Si heterostructure in darkness (*1*) and under illumination (*2*).

Photovoltaic effect in the obtained heterostructure was investigated using a xenon arc lamp of H3 type as a solar radiation simulator with a power of 35 W and a color temperature of 6000 K. The heterostructure was illuminated from the side of the film, the illuminance being 1800 lx. The radiation power density $p = 0.0024$ W/cm^2 was estimated from the lamp radiation power per unit of the area of the sphere with the radius equal to the distance from the lamp to the illuminates sample. The *I–V* characteristics of the studied heterostructures at direct current were determined by the standard two-contact method. The dark *I–V* characteristics were measured under the conditions of complete darkness in the absence of heat sources located nearby.

3. Result and discussion

The *I–V* characteristics obtained under the conditions of darkness and at the film illumination are presented in Fig. 1. The positive value of *U* corresponds to the polarity Si "–", SiC "+". Such a choice of the polarity of the external electric field is caused by the fact that the forward bias field reduces the contact field of the depleted layer. The direction of the contact

Table. Width of the forbidden band E_g and the electron affinity energy χ of the heterojunction-forming materials

	Si	21R–SiC
E_g	1.1 eV [9]	2.96 eV [10]
χ	4.05 eV [9]	3.5 eV [10]

field E_{intr} in the heterojunction is defined by the difference in the values of the work function φ of the materials which form the heterojunction. In the considered case $\varphi_{\mathrm{Si}} = \chi_{\mathrm{Si}} + E_{g(Si)} - \delta_{\mathrm{Si}}$, $\varphi_{\mathrm{SiC}} = \chi_{\mathrm{SiC}} + E_{g(SiC)} - \delta_{\mathrm{SiC}}$, where χ is the energy of electron affinity, δ_{Si} and δ_{SiC}, the energy gaps between the Fermi level E_F and the valence band edges E_V in Si and SiC. For the materials which form the heterostructure $\chi_{\mathrm{SiC}} + E_{g(SiC)} > \chi_{\mathrm{Si}} + E_{g(Si)}$ (Table). So, since at hole doping the Fermi level E_F is located near the valence band edge, it may be concluded that the work function φ in SiC will exceed the one in Si. Therefore, the holes located within the contact layer move from SiC to Si. In this connection the contact-adjacent silicon region acquires a positive charge, the one of silicon carbide is charged negatively, and the electric field E_{intr} in the contact layer is directed from Si to SiC.

Photovoltaic effect in the obtained heterostructure is characterized by the positive value of the open-circuit voltage V_{oc} = 225 mV and the short-circuit current I_{sc} = 1 mA. The filling factor of the I–V characteristic defined as the ratio $V_m I_m / V_{oc} I_{sc}$, where V_m and I_m are the voltage and current corresponding to the maximum power, is equal to 26 %. Photovoltaic effect in the external electric field shows a weakly pronounced I–V characteristic asymmetry, practically linear behavior of the dark I–V characteristic at the reverse bias of the heterojunction, the increase of photocurrent in the reverse bias fields followed by saturation (parallelism of curve *1* and curve *2* at $U < 0$) and the change of photocurrent direction at the forward bias (intersection of curve *1* and curve *2* at $U > 0$).

To explain the above peculiarities, there was proposed the following qualitative scheme of the energy bands of the considered heterojunction (Fig. 2). The values of the conduction and the valence bands offsets are $\Delta E_C = \chi_{\mathrm{Si}} - \chi_{\mathrm{SiC}}$ = 0.5 eV and $\Delta E_V = (E_{g(SiC)} - E_{g(Si)}) + (\chi_{\mathrm{SiC}} - \chi_{\mathrm{Si}})$ = 1.2 eV, respectively. Since the values of δ are considerably lesser than the energies of electron affinity and the forbidden band width both in silicon [11] and silicon carbide [12], the estimated contact difference of the potentials is

$$V_{intr} = [\varphi_{\mathrm{SiC}} - \varphi_{\mathrm{Si}}]/e \approx [(\chi_{\mathrm{SiC}} + E_{g(\mathrm{SiC})}) - (\chi_{\mathrm{Si}} + E_{g(\mathrm{Si})})]/e = 1.2 \text{ V}.$$

Thereat, while constructing the band energy diagram (Fig. 2) the quantitative ratios of the energy parameters were observed.

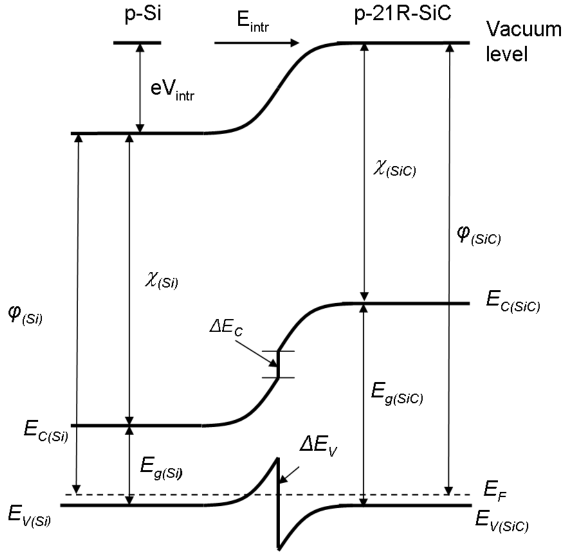

Fig. 2. Diagram of the energy bands of p–21R–SiC/p–Si heterojunction.

Since the holes are the main charge carriers in both layers of the heterostructure, the asymmetry of the dark I–V characteristic is caused by the differences in the potential barrier heights for the holes at the forward (the valence band bending is barrier) and reverse (the value ΔE_V is barrier) biases. As in the former case the barrier height exceeds the one in the latter case (Fig. 2) and the barrier for the holes at the forward bias diminishes, the current $I_{forw.} > I_{rev.}$. The value of the barrier ΔE_V connected with the valence band offsets is caused only by the values of the forbidden band width and the electron affinity of the semiconductors which form the contact layer, and do not depend on the external electric field. This gives rise to linearity of the dark I–V characteristic at the reverse bias.

The photoelectrons formed at illumination of the film will migrate from the contact-adjacent SiC region into the Si layer of the heterostructure under the influence of the contact field E_{intr}. As a result, the film is charged positively and the substrate is charged negatively, i.e. oppositely to the direction of the contact field, that corresponds to the experimentally observed positive sign of photo-emf. Due to the presence of the energy barrier in the valence band, photo-holes do not participate in the appearance of photovoltaic effect.

At the reverse bias $U_{rev.}$ the value of the field in the contact region rises and that leads to the increase of the photocurrent (the initial segment of the I–V characteristic at $U < 0$). With the increase of the external electric field corresponding to the reverse bias all the photoelectrons formed under the influence of light will move from the SiC layer to the Si layer of the heterostructure. In the experiment this manifests itself in saturation of the photocurrent value with the growth of $U_{rev.}$ (parallelism of the I–V characteristic of the darkened and illuminated heterostructure, Fig. 1). The forward bias of the heterojunction diminishes the band bending which decreases the energy barrier height both in the conduction and the valence bands. As a consequence, there appears an additional contribution to the current through heterojunction caused by the migration of photoelectrons from Si to SiC and of photoholes from SiC to Si. This photocurrent directed oppositely to the one in the absence of external electric field increases the value of the current through heterojunction at its forward bias: $I_2 > I_1$ at $U > 0.35$ V, Fig. 1.

4. Conclusion

Thus, after achieving the required electrophysical parameters of the considered isotype heterostructure p–SiC/p–Si, the latter may be of interest for solar power engineering. All the experimentally observed features of the I–V and photoelectrical characteristics are caused by the presence of potential barriers in the contact region caused by the band offset.

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Фотовольтаїчний ефект у гетеропереході p–SiC/p–Si

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Досліджено фотовольтаїчний ефект в ізотипному гетеропереході з дірковою провідністю, утвореному плівками нанокристалічного p–21R–SiC, осадженими на монокристалічні підкладинки з p–Si (гетероперехід p–SiC/p–Si). Плівки отримували методом прямого іонного осадження. Особливості вольтамперних та фотоелектричних характеристик гетероструктури p–SiC/p–Si пояснено впливом потенційних бар'єрів, зумовлених розривами зон у контактній області, на міграцію носіїв заряду через гетероперехід.