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SURFACE PHOTOVOLTAGE IN PHOTOEMISSION STUDIES AT Si/InP(110) HETEROJUNCTIONS*

B. ADAMOWICZ

Institute of Physics, Silesian Technical University
Krzywoustego 2, 44-100 Gliwice, Poland

C. OTTAVIANI, C. QUARESIMA AND P. PERFETTI

Istituto di Struttura della Materia/CNR, Via E. Fermi 38, 00044 Frascati, Italy

We discuss the surface photovoltage effect observed in photoemission experiment performed at room (300 K) and low (120 K) temperatures on Si/InP(110) heterojunctions for a thin Si coverage on *n*- and *p*-doped InP substrates. The theoretical analysis of the surface photovoltage effect has been performed on the basis of thermionic and thermionic-field emission models of transport processes in Schottky barriers.

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1. Introduction

The surface photovoltage phenomenon, i.e., a change in band bending induced by photons at semiconductor surfaces and interfaces with built-in potential barriers, has recently been observed in UPS experiments at many metal–semiconductor Schottky junctions [1] and only in a few cases of semiconductor–semiconductor interfaces [2, 3].

In Ref. [3] dell'Orto et al. have reported on the surface photovoltage at the a:Si/*n*-InP(110) heterojunction at 120 K, generated by ultraviolet synchrotron radiation in photoemission studies. It is interesting that for the junction with a *p*-InP substrate they did not observe any surface photovoltage effect (SPV). They described the SPV mechanism qualitatively in terms of generation, transport, and recombination of excess electron–hole pairs at the heterojunction. In this work we discuss those results on the basis of both the thermionic and thermionic-field emission models of transport phenomena in Schottky barriers [4, 5].

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2. Si/n-InP(110) heterojunction

The Si/n-InP(110) heterojunction was obtained by evaporation of 1 nm of a:Si on the InP(110) surface cleaved under UHV conditions (5×10^{-10} mbar) and studied *in situ* by means of photoelectron spectroscopy at 300 and 120 K [3]. A pronounced shift of 0.3 eV towards higher binding energies was observed in the UPS spectra measured at 120 K compared to the spectra at 300 K. This result was attributed to the non-equilibrium state (SPV) induced by the ultraviolet synchrotron radiation at the interface. Figure 1a illustrates this situation. Photoelectrons generated by UV radiation are driven away from the interface by the potential of the depletion layer, whereas photoholes go into the opposite direction.

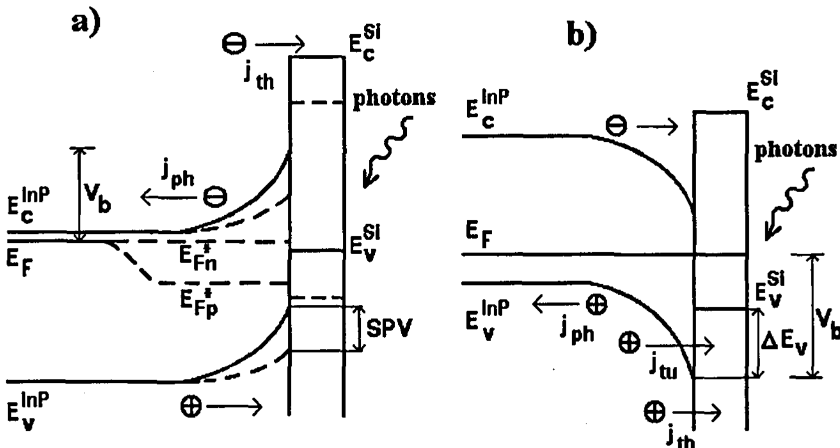

Fig. 1. Band structure of Si/n-InP (a) and Si/p-InP interfaces (b) in the dark (solid lines) and under illumination (dashed lines). In the case (b), SPV = 0, as in the experiment. The valence band discontinuity $\Delta E_v = 0.6$ eV [3]. The arrows point the excess carrier flows.

This photocurrent ($j_{\rm ph}$) is restored mainly by the thermionic emission current of electrons from InP to Si ($j_{\rm th}$) and then recombination at the interface. Another possible restoring process, the tunneling of electrons through the interface barrier from n-InP to Si, seems to be less probable because of the much lower density of electron states near the midgap of Si, where the tunneling can occur, than near the edges of the gap (U-shape distribution of the interface states). As a result, a partial flattening of the energy bands (SPV) appears. The surface photovoltage can also be measured in an UPS experiment as a shift in the Fermi level at the interface, i.e., a distance between the Fermi level in the dark ($E_{\rm F}$) and the hole quasi-Fermi level ($E^*_{\rm Fp}$) under illumination. The state of the shined heterojunction is similar to the forward-biased Schottky diode. Therefore, according to the thermionic emission theory, the photocurrent $j_{\rm ph}$ is given by the following formula [6]:

$$j_{\rm ph} = A^* T^2 \exp(-qV_{\rm b}/kT)[\exp(qV_{\rm ph}/kT) - 1], \qquad (1)$$

where $A^* = 4\pi m_n q k^2 h^{-3}$ is the Richardson constant of InP, m_n is the electron effective mass (for InP $m_n = 0.077 m_0$ [7], where m_0 is the free electron mass), k is the Boltzmann constant, h is the Planck constant, T is the temperature, q is the electron charge, V_b is a distance between E_c and E_F at the interface and V_{ph} is the surface photovoltage.

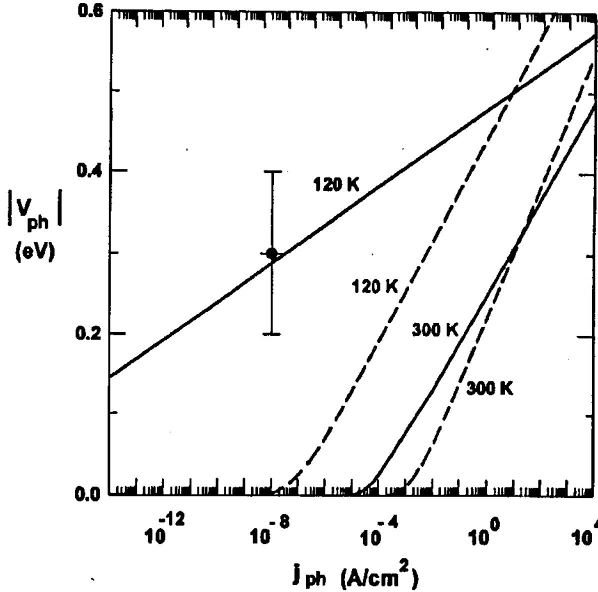

Fig. 2. Theoretical dependences of the absolute value of SPV vs. photocurrent density for Si/n-InP (solid lines) and Si/p-InP (dashed lines). The black circle represents experimental values of SPV and j_{ph} at 120 K for Si/n-InP; for Si/p-InP, SPV = 0.

The results of calculations of V_{ph} vs. j_{ph} at 120 and 300 K, on the basis of Eq. (1), and for $V_b = 0.6$ eV [8] are presented in Fig. 2 (solid lines). It is clear that the experimental values of V_{ph} (0.3 eV) and j_{ph} (estimated at about 10^{-8} A/cm^2), represented by the black circle in Fig. 2, are in good agreement with the theoretical curve. Moreover, we see the theoretical value of SPV at 300 K is about zero for $j_{ph} = 10^{-8}$ A/cm^2.

3. Si/p-InP(110) heterojunction

For the a:Si/p-InP heterojunction, contrary to the previous system, there was no shift in the UPS spectra (no SPV) at 120 K [3]. Figure 1b shows the band scheme of this heterojunction. The UV photons generate excess electrons and holes which are driven into opposite directions (j_{ph}). The restoring current consists of both the thermionic (j_{th}) and tunneling (j_{tu}) currents through the "notch" in the valence band. Therefore, the theoretical analysis of SPV was carried out on the basis of the thermionic-field emission theory [6]. The photocurrent j_{ph} is given by the formula

$$j_{ph} = j_{th} + j_{tu} = j_s \exp(V_{ph}/E_0)[1 - \exp(-qV_{ph}/kT)], \qquad (2)$$

where

$$E_0 = E_{00}\coth(qE_{00}/kT) \quad \text{and} \quad E_{00} = h/(4\pi)[N_\mathrm{d}/(m_p\varepsilon\varepsilon_0)]^{0.5}, \tag{3}$$

$$j_\mathrm{s} = j_\mathrm{m} q \frac{[\pi E_{00}(V_\mathrm{b} - V_\mathrm{ph} - V_n)]^{0.5}}{[kT\cosh(qE_{00}/kT)]} \exp[-(V_\mathrm{b} - V_n)/E_0] \tag{4}$$

and

$$j_\mathrm{m} = A^* T^2 \exp(-qV_n/kT). \tag{5}$$

In Eqs. (2)–(5) m_p is the hole effective mass, ε and ε_0 are the semiconductor and vacuum permittivities (for InP $m_p/m_0 = 0.64$ and $\varepsilon = 12.61$ [7]), V_b and V_n are the separations between E_F and E_v at the interface and in the bulk of InP, respectively, and N_d is the acceptor concentration ($N_\mathrm{d} = 1.6 \times 10^{19}$ cm^{-3}). Using the relations given above and assuming $V_\mathrm{b} = 0.8$ eV [8], we calculated the dependences of V_ph vs. j_ph (dashed curves in Fig. 2). It is clear that at both 300 and 120 K, for $j_\mathrm{ph} = 10^{-8}$ A/cm^2, the value of SPV is about zero, as in the experiment.

The analysis presented indicates the differences in the restoring process of photon-induced charges at Si/InP(110) heterojunctions with n- and p-doped substrates. In the case of n-InP, the thermionic current of excess electrons from InP to Si prevails whereas in the case of p-InP the tunneling of holes through the potential "notch" is crucial. A more detailed analysis of these processes, including recombination at the interface, we will discuss in a future paper.

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