Proceedings of the XXIII International School of Semiconducting Compounds, Jaszowiec 1994

BAND-OFFSET AND ELECTRONIC PROPERTIES OF TYPE II PbTe/PbS SUPERLATTICES*

F.F. SIZOV, J.V. GUMENJUK-SICHEVSKAYA, V.V. TETYORKIN AND V.V. ZABUDSKY

Institute of Semiconductor Physics of the National Ukrainian Academy of Sciences
252028, pr. Nauki 45, Kiev, Ukraine

Semimetallic conductivity was observed in PbTe/PbS SL obtained by a "hot wall" technique on (001) KCl substrates with (001) PbTe buffer layers. From the analysis of $R_H(H)$ and $\rho_\perp(H)$ dependencies by the Monte-Carlo fitting procedure the band offset $\Delta E_v = 0.32 \pm 0.05$ eV was obtained ($T = 77$ K) and it was proved that these SLs are type II "misaligned" structures. The calculations of the band structure of PbTe/PbS SLs showed that in such SLs a semimetal–semiconductor transition should occur for layer thicknesses of about 60÷70 Å.

PACS numbers: 68.65.+g

Investigated up to now IV–VI superlattices (SLs) as a rule belong to type I SLs [1] except PbTe/SnTe system which forms type II "misaligned" SL [2]. Type II SLs offer some interests for infrared (IR) detector applications as it is possible to realize in such kind of systems favorable optical properties for long-wavelength detector applications through the valence to conduction band optical transitions between the states in alternate layers due to overlap of the envelope wave functions (see, e.g. [3]). The band gap in such structures occurs between the electron states localized in one types of layers and the hole states localized in remaining layers. PbTe/SnTe type II SLs however could not be used as effective photodetectors because of very high hole concentrations inherent to SnTe layers. It is supposed that type II IV–VI SLs also can be realized in PbTe/PbS system, as these semiconductors differ much by the affinity energies ($\chi_{PbTe} = 4.6$ eV [4], $\chi_{PbS} = 3.9 \div 4.2$ eV [5]).

PbTe and PbS compounds differ much by the lattice constants ($a_{PbTe} = 6.460$ Å and $a_{PbS} = 5.94$ Å) that should cause the arising of misfit dislocations at the interface. But as it was earlier shown for this system [6] the misfit dislocations are generated only in a thin layer near the interface. Beyond this thin highly deteriorated layer with "wood" of dislocations [6] the layers are unstrained and one can suppose to obtain the perfect layers with good electrical characteristics.

*This work was partly supported by the grant No. 2.2/11 from the Ukrainian Committee of Science and Technology.

PbTe/PbS SLs with the number of periods up to $N = 100$ were prepared by the "hot wall" epitaxy technique in a vacuum chamber with the gas pressure of $10^{-5} \div 10^{-6}$ torr at substrate temperatures not exceeding $T = 350°C$. In this temperature range the metallurgical boundary between the PbTe and PbS layers should be very pronounced due to the absence of the intermixture between the constituents at temperatures $T < 400°C$. The presence of the misfit dislocations at the interface in PbTe/PbS system also prevail the intermixture of the components [6].

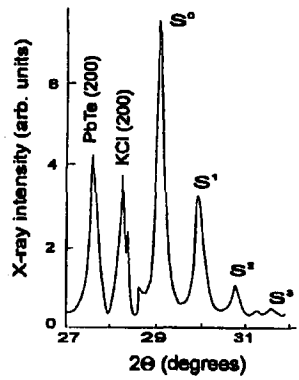

Fig. 1. Experimental X-ray spectra of 100-period PbTe/PbS (60 Å/60 Å) SL on KCl substrate with $d \approx 1$ μm PbTe buffer layer.

The SLs grown exhibit up to four regularly spaced X-ray SL satellites (see Fig. 1). The appearance of numerous sharp, regularly spaced X-ray satellites is an indication of high structure quality SLs with little constituents interdiffusion [7]. Growth of SLs commenced with deposition of $(10^3 \div 10^4)$ Å buffer PbTe or PbS layers a top of the (100) KCl substrates. The thickness of PbTe or PbS layers in SLs varied between 60 and 500 Å. The total thickness of PbTe/PbS SLs with buffer layers was in the range of $2 \div 3$ μm.

Studies of the angle dependencies of transverse magnetoresistance showed a very pronounced epitaxy technique and confirmed quasi-two-dimensional character of conductivity in PbTe/PbS SLs.

Up to now the band offset in PbTe/PbS is not established. To obtain the quantitative values of band offset in these objects the studies of the temperature and magnetic field dependencies of Hall coefficient and transverse magnetoresistance were carried out.

To analyze the experimental dependencies in PbTe/PbS SLs the multilayer conductivity model [8] was applied and the Monte–Carlo fitting procedure was used to find the equations solutions for this multilayer conductivity model.

The Monte–Carlo simulation method has been chosen to find the solution of the system of equations for transverse magneto-resistance and the Hall coefficient for multilayer structure [8]

$$\frac{\rho_\perp}{\rho_0} = \frac{\sum_i d_i N_i \mu_i(0)}{\sum_i d_i N_i \mu_i(H)} \left[1 + (\mu_H H)^2\right],$$

$$R_H = \rho_\perp(H)\mu_H, \tag{1}$$

where the Hall mobility of a structure with different types of carriers in layers is determined by the expression $\mu_H = \sum_i d_i N_i \mu_i^2(H) / \sum_i d_i N_i \mu_i(H)$. The values of carrier mobilities $\mu_i(H)$ and $\mu_i^2(H)$ in the magnetic field are defined by $\mu_i(H) = \langle \mu_i(0)/(1 + \mu_i^2(0)H^2) \rangle$, $\mu_i^2(H) = \langle \mu_i^2(0)/(1 + \mu_i^2(0)H^2) \rangle$.

Experimentally determining the layer thicknesses and the resistivity, it is possible to obtain the basic electrical characteristics of each separate layer in the multi-layer structure, such as carrier concentrations of each SL layer N_i and their mobilities μ_i from experimental $R_H(H)$ and $\rho_\perp(H)$ dependencies (Eq. (1)) [8] by the Monte–Carlo fitting procedure.

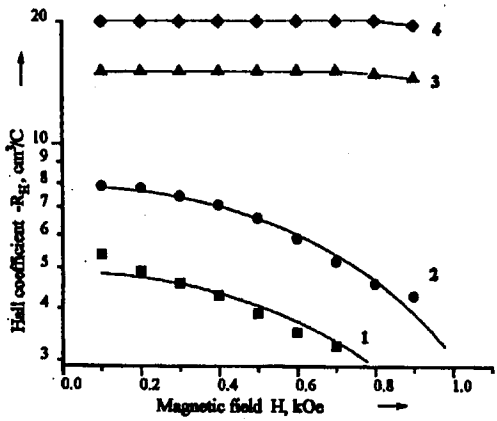

Fig. 2. Magnetic field dependencies of the Hall coefficient. (1, 2) — PbTe/PbS SLs, (3) — PbS film, (4) — PbTe/PbS (1.5 μm/1.5 μm) heterostructure.

The Hall coefficient and magnetoresistance dependencies on magnetic field were measured for PbTe/PbS SLs, PbS film and one PbS/PbTe heterostructure (see Fig. 2). There exists an essential difference in magnetic field dependencies for SLs, films and heterostructures. For last two objects there is almost no $R_H(H)$, $\rho_\perp(H)$ dependencies which is characteristic for films and heterostructures in the case of in-plane transport. For SLs the $R_H(H)$ and $\rho_\perp(H)$ dependencies are very strong even in weak magnetic fields which is characteristic for systems with two types of carriers (electrons and holes) with different mobilities (see e.g. [9]).

The Monte–Carlo simulation procedure can be fitted with the experimental data only in the case, when in PbS there are holes and in PbTe there are electrons. In these growth conditions used the separate PbS or PbTe layers were grown only of n-type conductivity. Thus, the change of the conductivity type in PbS layers, when they form a SL with PbTe layers, can be only in case when the electrons from PbS layers overflow to PbTe layers. It is possible only in case when these materials form a type II "misaligned" structure, and so the top of PbS valence

band is above the bottom of the PbTe conduction band. Then, calculating the position of the Fermi level in the SL one can obtain the band-offset (ΔE_v) in this system. The valence band offset obtained $\Delta E_v = 0.32 \pm 0.05$ eV.

Using the values of the band-offset obtained, the band structure of PbTe/PbS SLs was calculated. The band structure calculations of PbTe/PbS SL with [100] growth direction were made in the envelope-function approximation [10] taking into account the nonparabolicity of the components bands near extremal L-points of the Brillouin zone in the framework of two-band Kane model.

We have calculated the band spectra of PbTe/PbS SL for different layer thicknesses and for temperatures $T = 77$ and 300 K. For layer thicknesses greater than 60 Å the PbTe/PbS SL without the buffer layer must exhibit a semimetallic conductivity due to the hybridization of s-type valence band states of PbS and p-type conductivity band states of PbTe at $T = 77$ K. At higher temperatures the overlap decreases, and the transition to the state with the semimetallic conductivity must occur at higher layer thicknesses for the SL without the buffer layer. The presence of the buffer layer changes the situation, as for any PbTe layer thicknesses and for PbS thicknesses ≥ 35 Å there would always be the n-type conductivity in PbTe buffer layer and the p-type conductivity in PbS SL layers. Thus such kind of a system will be a semimetallic one.

For the thicknesses $a \simeq b \leq 60$ Å the PbTe/PbS SL itself must go over to the semiconductor one and can be used for the design of IR-photosensitive structures. Estimations of the interband absorption coefficient α have shown that $\alpha \simeq 10^3$ cm^{-3} at wavelength cutoffs of about 10 μm, which is a sufficient value for IR-photodetector applications.

The optical absorption spectra of PbTe/PbS SLs investigated in this work did not reveal any SL absorption, as this to be observed, one need to have the SL with the period smaller than 120 Å as to have the PbS valence band states lower than the PbTe conduction band states. But SLs with $d \leq 120$ Å were not obtained by the "hot wall" technique due to rather large layers growth rates (≤ 8 Å/sec) and inertia of the growth system used, which does not allow one to obtain the thin layers (< 60 Å) with great accuracy needed for this case.

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