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(001)-oriented lead selenide films grown on silicon substrates

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Abstract

Lead selenide epitaxial films were grown on silicon substrates using a thin (≤ 100 nm) YbS buffer layer. The films were (001)-oriented and had structural, electrical and photoelectrical properties comparable with those of PbSe bulk crystals. The X-ray rocking curve halfwidths were of 100–200 arcsec which are within similar values for PbSe/BaF₂(CaF₂)/Si films, thoroughly investigated for infrared detector array applications. The films investigated exhibit relatively large photosensitivity in the temperature range $T = 80$ –300 K. Minority carrier lifetime values $\tau \approx 10^{-6}$ s at 80 K and their temperature dependencies are preferably determined by the Shockley–Read–Hall recombination mechanism through the deep levels in the band gap.

1. Introduction

There is a range of different infrared (IR) detector materials which can find applications in large scale detector arrays. But it is possible to use only few of them in focal plane arrays (FPA), operable at room temperature or at temperatures which are compatible with long-lived low cost coolers. The FPA should preferably be arranged completely on a Si substrate in order for low power readouts to be used. Presently most of the work is connected with mercury–cadmium–telluride alloys grown on CdTe or CdZnTe substrates and connected with Si readout devices [1,2].

Despite the fact that HgCdTe alloys are the most usable materials for manufacturing of IR detection

systems such as focal plane arrays, heteroepitaxy of IV–VI narrow gap semiconductors on silicon substrates is also of great importance for IR optoelectronic applications [3–5]. The possibility exists in this case to manufacture fully monolithic detection systems. Compared to HgCdTe alloys IV–VI semiconductors have some advantages such as higher compositional uniformity due to a less pronounced dependence of the bandage on composition, material stability at elevated temperatures, relatively well behaved metallurgy which allows for the use of a large amount of growth procedures, including such a simple one as the thermal evaporation of thin films.

Direct epitaxy of IV–VI narrow gap semiconductors on Si substrates seems to be impossible due

respectively. A more pronounced difference between the films grown on the different substrates was established from X-ray topography measurements. It has been found that the layers grown on (001) KCl substrates consist of monocrystalline blocks with typical dimensions ranged from 10 to 40 nm. This result is in agreement with those obtained previously for IV–VI compounds [6]. However, it has been found that the films grown on (001) Si substrates covered with YbS buffer layers consist only of single monocrystalline blocks that have the same dimensions as the substrates (typically 3.0×8.0 mm).

The films with standard Hall configuration were prepared to measure their electrical properties using the conventional dc technique. Typical temperature dependencies of the Hall coefficient R_H are shown in Fig. 1. All the films prepared were of n-type conductivity. At 77 K the electron concentration is changed from 2×10^{17} to $1 \times 10^{18} \text{ cm}^{-3}$. Most of the films investigated have values of the electron mobility ranging from 10^3 to $10^4 \text{ cm}^2/\text{Vs}$ at $T = 77 \text{ K}$. The highest mobility values observed were of $1.5 \times 10^4 \text{ cm}^2/\text{Vs}$. These values are almost as high as those of bulk crystals [7,8]. The mobility decreases with temperature increasing with the power law $T^{-\beta}$, where $\beta = 2.3\text{--}2.5$. In this temperature range the carrier mobility can be explained as being due to scattering on both acoustical and optical phonons.

A pronounced decrease of the Hall coefficient is observed at temperature $T > 90 \text{ K}$. It cannot be explained by the temperature variation of the scattering factor [8,9] as well as by the influence of inhomogeneities in the layers. It seems that the dependence of R_H on temperature results from carrier freeze-out on the states in the band gap. At low temperatures, $T < 90 \text{ K}$, the Hall coefficient is seen to be temperature independent.

A few models of deep defect states have been examined to carry out numerical calculations of the carrier concentration. These include singly- and doubly-ionized defect states in undoped lead selenide films as well as in single crystals [10–12]. However, the best agreement between the measured and calculated data was obtained for a model considered in Ref. [13]. In accordance with this model the carrier concentration temperature

dependence in IV–VI compounds can be described by the expression

$$n = n_0 + 2N(1 - f), \tag{1}$$

where

$$f = f_{\frac{1}{2}} + f_{\frac{1}{2}}f_2. \tag{2}$$

Here the functions $f_{\frac{1}{2}}$ and f_2 are Fermi distribution functions with degeneracy factors $\frac{1}{2}$ and 2 respectively. In the case of PbSe/YbS/Si films the energy of the states in the gap $E_{dl} = -(30 + 0.14 T) \text{ meV}$ was assumed to describe best of all the experimental data $n(T)$ in the temperature range $T = 77\text{--}300 \text{ K}$. This value of the energy for deep levels (as compared to the band-gap of PbSe) is close to that obtained in Ref. [11] for PbSe/BaF₂ films. The densities of states N were found to be in the range of $2 \times 10^{18} \text{ cm}^{-3}$ to $5 \times 10^{18} \text{ cm}^{-3}$ in the films investigated. When describing the $n(T)$ experimental data the Fermi level temperature dependence was taken into account in the two-band nonparabolic approximation. For all the samples considered it happened that the electrons in the PbSe conduction band were in the state of intermediate degeneracy in the temperature range used.

In Eq. (1) n_0 stands for the concentration of carriers which cannot freeze-out. The lack of the carrier concentration dependence on T at low temperatures is typical for IV–VI compounds [8,13]. These unfreezing carriers are introduced into the conduction band due to the existence of resonant states [14–16]. The value of n_0 was

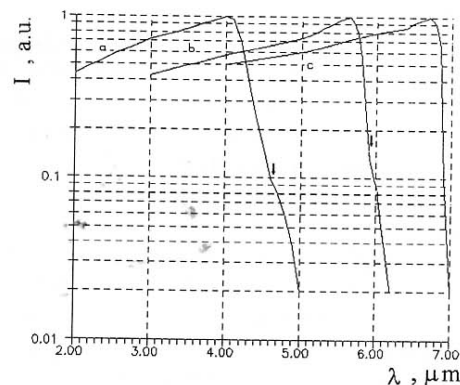


Fig. 2. Normalized photoconductivity spectra of a PbSe layer I measured at 300 (a), 158 (b) and 82 (c) K. The positions of the bandgap are indicated by arrows.

electron gas they can be used only as estimations. A more rigorous account of degeneracy in some IV–VI semiconductors was given in Refs. [19,20]. Despite the fact that at $T = 80$ K the calculated value of the Auger lifetime is closed to the measured one for a sample with electron concentration $n = 2 \times 10^{17} \text{ cm}^{-3}$, the temperature dependence of the carrier lifetime can hardly be explained by this recombination mechanism. Furthermore, the dependence of the lifetime on electron concentration seems to be less pronounced than that predicted by Emtage theory $\tau \sim 1/n^2$ as well as by the theory developed in Refs. [19,20].

Also shown are the radiative lifetime data calculated by the formula (15) from [19]. The temperature dependence of the radiative recombination time is very similar to that observed experimentally but the calculated data are more than an order less than the experimentally observed ones. Thus, this mechanism of carrier recombination also seems to be not very important in the objects considered.

As with temperature growth the carriers from the deep level E_{d1} are thermally generated to the conduction band, the SRH recombination via this level should be strengthened and the lifetime should be larger than at low temperatures when the level is completely filled. If the SRH recombination through the states in the gap, which were observed from the Hall effect measurements, takes place, one can estimate a minority carrier cross section $\sim 10^{-19} \text{ cm}^2$ at $T = 80$ K for the density of deep defect states $N \cong 10^{18} \text{ cm}^{-3}$. This value is in agreement with the data obtained previously [11].

The nature of deep defect states in undoped lead selenide bulk crystals and epitaxial layers is not clear yet. The experimental results obtained in this study are similar to those reported earlier. First of all, the relatively high density of the deep defect states in the gap $N \geq 10^{18} \text{ cm}^{-3}$ was obtained both in epitaxial films and single crystals [11,12,17]. These values of N exceed the concentration of uncontrollable impurities in the starting material (in this study it was estimated to be less than 10^{17} cm^{-3}). The most reasonable explanation of the values of N seems to be the vacancy states due to deviation from the stoichiometry, as point defects in both sublattices are electrically active and introduce the states in the gap and also in the conduc-

tion and valence bands [14,15]. In contrast to the one-electron model of [14] it was shown in the analytical tight-binding model [15] that one of the vacancy levels can be in the PbSe gap.

3. Conclusion

High quality PbSe monocrystalline films were grown on (001)-oriented Si substrates. YbS buffer layers with a thickness of $\sim 10^2$ nm were previously deposited onto Si substrates. The films grown on YbS buffer layers are composed of single monocrystalline blocks with dimensions as large as in Si substrates and exhibit both interband and impurity photoconductivity in the temperature range from 80 to 300 K.

The deep localized states in the gap near the conduction and valence band edges have been observed in n -type PbSe films grown on (001)-oriented Si substrates. The states under the conduction band minimum with the energy E_{d1} determine the temperature dependence of carrier concentration and non-equilibrium carriers lifetime. Another type of deep states (with energy E_{d2} above the valence band minimum) determine the spectral dependence of the photoconductivity spectra (impurity branch). The most probable reason for the deep defect states E_{d1} in the gap is the deviation from the stoichiometry.

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