Optical studies of wide-bandgap HgCdTe material used in potential- and quantum-well structures

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Abstract. Optical transmission and photoluminescence were used for the study of wide-bandgap (0.8-1.1 eV) HgCdTe (MCT) material grown by molecular-beam epitaxy. The material, including layers used as spacers and barriers in potential- and quantum-well structures, showed a considerable degree of alloy disorder similar to narrow-gap MCT grown by the same method. In some samples, defect states in the bandgap were found. Optimization of the growth technology for wide-bandgap material should help improving the quality of MCT-based potential- and quantum-well structures designed for various applications.

1. Introduction

For more than 50 years, Hg₁₋ₓCdₓTe (MCT) solid solutions have remained one of the basic materials for infrared (IR) photo-electronics. Up to recently, the most widely studied MCT was a narrow-gap material with chemical composition (CdTe molar fraction) x ≤ 0.4, as its bandgap $E_g$ corresponded to the energy of photons in long- (8 – 14 μm) and middle-wavelength (3 – 5 μm) IR ranges [1]. Presently, MCT with $x \approx 0.5$ also attracts considerable interest due to the development of photodetectors for so-called ‘extended Short–Wave IR’, eSWIR range (wavelengths $\lambda = 1.7 – 3.0 \mu m$) [2]. At the same time, MCT with $x \geq 0.6$ has not been studied in detail, as photo- and optoelectronic devices operating in the wavelength range corresponding to the bandgap of this material (0.8 – 1.6 eV at 300 K) can be easily made of less expensive and more technology advanced III-V semiconductors. Properties of wide-bandgap MCT were mostly studied at the early stages of the existence of the material in order to assist the development of its growth technology [3–6].

Recently, HgTe/Cd(Hg)Te quantum wells (QWs) have been studied intensively due to their unique properties and the resulting applications. HgTe/Cd(Hg)Te QWs with normal band ordering are of great interest for far-infrared opto- and photo-electronics and terahertz photonics [7], and QWs with the inverted band ordering (with QW wider than 6.1 nm for the HgTe/CdTe system) are extensively studied as topological insulators [8]. While much effort is put into producing QW structures with sharp interfaces and lack of composition gradient in the constituting layers [9], the structural and optical properties of barrier layers and spacers generally remain out of sight of the technologists and researchers. The quality of these layers is, however, very important, as it may affect optical and electronic properties of the final devices. These layers are commonly made of MCT with $x \approx 0.7 – 0.8$ [10], so we considered it worthwhile to study the optical properties of this material.
2. Experimental details
We studied epitaxial films (EFs), multi–QW (MQW, with a well width < 10 nm) and single potential-well (SPW, with well widths from 50 to 200 nm) structures containing MCT layers with $x = 0.68 - 0.78$. SPW double heterostructures did not show size quantization effects in optical experiments [10]. The samples were grown by molecular-beam epitaxy (MBE) on (013)GaAs substrates with ZnTe and CdTe buffer layers as described elsewhere [11,12]. Optical transmission (OT) and photoluminescence (PL) were used in the studies. OT spectra were recorded at 300 K with the use of an Infralum-801 Fourier-Transform IR spectrometer. PL spectra were recorded in the 4.2 – 300 K temperature range with the use of an MDR-23 grating monochromator. The PL signal was excited by a semiconductor laser with a wavelength of 1.03 µm and was registered with a Ge photodiode that cut out long-wavelength PL coming from the narrow-gap wells. Optical properties of some of these wells were reported elsewhere [10].

For comparison, we also studied an EF grown by liquid-phase epitaxy (LPE). The film was grown in a closed-system LPE machine from Te-rich melt on a (111)CdZnTe substrate. After the growth, the film was thermally annealed in saturated Hg vapours at 230°C for 48 hours for attaining n-type conductivity. Parameters of the studied samples are given in table 1. The composition $x$ and the thickness of the MBE-grown film and layers were assessed with the use of in situ ellipsometric measurements [11,12], those of the LPE-grown film, with OT and optical microscopy.

| Sample | Structure type (well widths) | Growth method | $x$ in the studied layer(s) | Number $\times$ thickness of the studied layer(s), nm |
|--------|-------------------------------|---------------|----------------------------|-------------------------------------------------|
| $A$    | SPW (1×200)                  | MBE           | 0.68                       | 2×1000                                           |
| $B$    | EF                            | LPE           | 0.69                       | 10300                                           |
| $C$    | MQW (11×7.1)                 | MBE           | 0.70                       | 2×4000                                           |
| $D$    | EF                            | MBE           | 0.72                       | 5000                                            |
| $E$    | SPW (1×50)                   | MBE           | 0.75                       | 2×1000                                           |
| $F$    | SPW (1×200)                  | MBE           | 0.78                       | 2×1000                                           |

3. Experimental Results and Discussion
Figure 1(a) shows OT spectra of some of MBE-grown samples recorded at 300 K. As can be judged from the OT edge, the transmission in PW and MQW samples at room temperature was determined by barrier (spacer) layers. In contrast to that, the photocconductivity of these samples at both 300 and 77 K (spectra not shown) was determined by the carriers in the wells. The OT spectra appeared to be typical of MBE-grown MCT. They showed reasonably sharp transmission edges and pronounced interference fringes at low wavenumbers, which were indicative of a good structural quality of the material. The values of $x$ in the material, estimated from the wavenumber corresponding to 50% OT, appeared to be slightly lower than those determined with ellipsometry. For film $D$, both the OT and ellipsometry data showed the presence of two layers with different compositions, which were determined with the use of OT as 0.70 and 0.74, respectively.

Figure 1(b) shows the PL spectra of samples $A$, $E$ and $F$ recorded at 85 K. The spectrum of sample $E$ represented a single band with a full-width at half-maximum (FWHM) of 52 meV. The spectra of samples $A$ and $F$ clearly consisted of two bands separated by 40 and 60 meV, respectively. The FWHMs of the high-energy bands (’edge PL’ bands) were ~ 50 meV. A defect-related PL band separated from the high-energy band by 40 to 70 meV is not typical of MCT grown by MBE on GaAs substrates but is often observed in the material grown on Si substrates [13]. The PL spectra of samples $A$, $E$ and $F$ recorded at 300 K (not shown) represented single bands with FWHMs from 60 to 65 meV.
Figure 2(a) shows the normalized PL spectra of samples B, C and D recorded at 85 K. The spectrum of the LPE-grown film B represents a symmetrical narrow band with a FWHM of just 17 meV.

**Figure 1.** Room-temperature optical transmission spectra of samples A, C, D and E (a), and normalized photoluminescence spectra recorded at 85 K for samples A, E and F (b) with thin lines showing fitting and decomposition of the spectra.

The spectra of the MBE-grown film and layers were much broader; their shape was slightly distorted by the absorption by gases present in the atmosphere. The PL spectrum of the MBE-grown film D at 85 K contained two bands with a FWHM of the high-energy band being 37 meV, while the spectra of the barrier layer of MQW sample C was broader with a FWHM of ~ 50 meV. In the MQW structure, the thicknesses of the barriers between the QWs was 25 nm, so one could expect that most of the laser emission was absorbed not by the barriers, but by much wider spacers, whose parameters are given in table 1. Still, some broadening of the spectra in the MQW and SPW structures could be attributed to the presence of a number of layers with similar, yet slightly different, chemical compositions.

**Figure 2.** Normalized PL spectra of samples B, C and D recorded at 85 K (a), and PL spectrum of sample D recorded at 4.2 K with thin lines showing fitting of the spectrum and its decomposition (b).

Figure 2(b) shows the normalized PL spectrum of sample D recorded at 4.2 K. As can be seen, the spectrum can be easily decomposed into three bands. Variable-temperature PL measurements showed that while the weak mid-energy band (probably, defect-related) blended into the strong low-energy one at ~ 80 K (see figure 2(a)), the existence of the low- and high energy bands could be traced up to 250 K. Figure 3 shows the temperature dependences of the positions of the maxima of these bands $E_{pl}(T)$, and the $E_g(T)$ dependence calculated for $x = 0.68$ in accordance with the empirical $E_g(x,T)$ relation from reference [14]. The low- and high-energy PL bands demonstrate different signs of
$dE_{PL}/dT$, which confirms the presence of two layers with different chemical compositions (in PL experiments, HgCdTe with $x$ up to -0.65 can show a positive ‘$dE_{PL}/dT$’ sign [3,4,13]). A gap between $E_{PL}(T)$ of the high-energy band and $E_g(T)$ at $T < 100$ K is due to the fact that the optical transitions responsible for this band were caused by recombination of excitons localized at compositional fluctuations [3–6].

Recent transmission electron microscopy studies of MCT QW structures showed good quality of the material of the barrier and spacer layers with respect to structural defects [15]. Thus, the substantial broadening of the PL spectra of the material grown by MBE as compared to that grown by LPE suggests a considerable degree of alloy disorder, similar to that in MBE-grown MCT with a lower CdTe molar fraction [13]. It has been noted that, while according to the general concept that considers a purely stochastic distribution of atoms over different sites of the crystal lattice, the maximum disorder should be observed at $x = 0.50$, in MBE-grown MCT this was not the case, which implied the presence of some technology-related disorder [13]. Thus, it seems that the technology of wide-bandgap MCT needs optimization, so compositional fluctuations related to the synthesis issues could be brought down to the level of purely stochastic fluctuations. This should help to improve the quality of the barrier and spacer layers in MCT-based quantum-well structures and their resulting properties.

4. Conclusion
In conclusion, using optical transmission and photoluminescence, we have studied optical properties of wide-bandgap (0.8 - 1.1 eV) HgCdTe (MCT) films and layers. We have found that the wide-gap MCT grown by MBE possesses a considerable degree of alloy disorder, similar to the material with a lower CdTe molar fraction grown by the same method. Also, in some samples, defect states in the bandgap were found, which is generally not typical of MCT films grown on GaAs substrates. There is certainly some room for improvement in relation to MBE of MCT with a high CdTe molar fraction, and optimization of this technology can be expected to help improving the quality of MCT-based quantum-well structures, which are currently of great demand.

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