Excitation density dependence of the photoluminescence from Cd$_x$Hg$_{1-x}$Te multiple quantum wells

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Abstract. A study of the photoluminescence from a four-period Cd$_x$Hg$_{1-x}$Te multiple quantum well structure at 11 K as a function of excitation density is presented. High-resolution X-ray diffraction and transmission electron microscopy revealed that the quantum well structure is of high quality. This was supported by the narrow photoluminescence peak originating in the ground state electron - heavy hole transition, with a full width at half maximum of only 7.4 meV for an excitation density of 1.3 W/cm$^2$. When the excitation density was increased from 1.3 to 23.4 W/cm$^2$, the peak position was shifted toward higher energy by 2.6 meV and the full width at half maximum increased from 7.4 to 10.9 meV.

1. Introduction

Cd$_x$Hg$_{1-x}$Te (CMT) is an important material for the fabrication of infrared detectors [1, 2] as the bandgap, which is direct for all Cd mole fractions, can be tuned from -0.26 eV in the semimetal HgTe ($x = 0$) to 1.61 eV in CdTe ($x = 1$) at 77 K [3]. Over the entire Cd mole fraction range, the lattice mismatch is maximum 0.3%. This allows heterostructures, including quantum well structures, to be made without considering strain effects. In quantum well structures, the energies of the discretely quantized energy levels are determined by both the composition in the well and barrier layers and the thickness of the well layer. The emission wavelength of a CMT quantum well light emitting device can hence be tuned either by varying $x$ or by varying the well thickness, in contrast to a bulk device where the emission wavelength can be tuned only compositionally. The emission spectra of quantum well structures are useful as they provide information not only about the quantized energy levels, but also about the crystal quality and the layer interfaces. Photoluminescence (PL) spectra from CMT multiple quantum well (MQW) structures have been presented by several groups [4–7]. However, a study of the position and width of the PL peak as a function of excitation density has, to our knowledge, not yet been presented. In this paper, the PL peak position and full width at half maximum (FWHM) as functions of excitation density are investigated.
2. Experimental
The Cd$_x$Hg$_{1-x}$Te/ Cd$_y$Hg$_{1-y}$Te MQW structure contained four periods and was grown by molecular beam epitaxy (MBE) in a 32P Riber machine on a (211)B CdZnTe 15mm×15mm substrate. Four material sources were used during growth: a Riber MCL160 Hg source, a low temperature SUMO source from Veeco for Te, and two standard CdTe sources. All four sources were open during deposition of the barrier layers, while the well layers were grown by closing the shutter in front of one of the CdTe sources. The substrate was Ga-bonded to the substrate holder, and the growth temperature was measured using a spring-loaded, Ga-wetted thermocouple in contact with the back of the substrate holder [8]. This setup provides good thermal contact between the substrate and the thermocouple even when the substrate is rotated during growth. The MQW structure was grown on top of a 4 µm buffer layer of the same composition as the well layers, and this allowed the Cd mole fraction of the well layers to be determined by means of transmission spectroscopy. An IFS 66 Fourier-transform spectrometer from Bruker was used for both the transmission and the PL spectroscopy. In order to avoid features from atmospheric absorption in the spectra, the entire beam path was flushed with N$_2$. Electron-hole-pairs were only excited in the buffer and well layers as the laser (617 meV) had lower energy than the bandgap of the barrier layers. The average lattice parameter in the growth direction and the total thickness of one well and one barrier layer were measured using high-resolution X-ray diffraction (HRXRD) in order to be able to determine the Cd mole fraction in the barrier layers and the thicknesses of both the well and the barrier layers. The HRXRD machine was a Philips PW 1880 with a four-crystal Ge monochromator. A Jeol 2010 F transmission electron microscope (TEM) was used to examine the crystal quality of the MQW sample.

3. Results and discussion
The results from transmission spectroscopy and HRXRD revealed that the Cd mole fraction in the well (barrier) layer was 0.36 (0.61), while the well and barrier layer thicknesses were 9.2 and 29.7 nm, respectively. A simulated HRXRD spectrum, together with the measured spectrum, are shown in figure 1. The presence of Pendellösung fringes between the satellite peaks in the measured spectrum, in addition to the good agreement between the measured and the simulated spectrum, indicate good interface quality in the MQW structure. This is confirmed by the high-resolution TEM image in figure 2(a) showing two well/barrier interfaces indicated by the white lines. The positions of the interfaces were extrapolated from an area further away from the ion-milled hole in the sample. Figure 2(b) shows a diffraction pattern and figure 2(c) shows a bright field overview image of the MQW structure, the high-x barriers appearing as light areas and the lower-x buffer and well layers appearing darker.

The PL spectra at 11 K contained two peaks separated by approximately 70 meV, where the low- and high-energy peak were attributed to the buffer layer and the ground state electron - heavy hole ($e_1hh_1$) transition in the MQW structure, respectively.
Figure 3 shows the PL peak originating in the $e_1hh_1$ transition at 11 K for excitation densities from 1.3 to 23.4 W/cm$^2$. The inset shows a magnification of the peak resulting from the lowest excitation density with a FWHM of only 7.4 meV which is, to our knowledge, the lowest FWHM reported for a CMT MQW. The evolution in peak position (open circles) and FWHM (closed circles) with excitation density are shown in figure 4. The peak position is shifted toward higher energy by 2.6 meV and the FWHM is increased from 7.4 to 10.9 meV when the excitation density is increased from 1.3 to 23.4 W/cm$^2$. The distribution of transition energies contributing to the $e_1hh_1$ PL peak is hence both shifted toward higher energy and widened when the excitation density is increased.

The temperature was measured on the back of the sample and remained fixed at 11 K for all excitation densities. However, the surface temperature and hence the temperature gradient in the growth direction are expected to have increased with increasing excitation density. Since the effective bandgap of the MQW structure increases with temperature, this leads to a shift in the PL peak position toward higher energy. Assuming that the surface temperature was close to 11 K at the lowest excitation density, calculations using a simple finite square well model predict that the surface temperature would have to be approximately 32 K at the highest excitation density for the peak position to be shifted by 2.6 meV. Broadening of the peak due to non-uniform temperature in the volume from which the photons contributing to the $e_1hh_1$ peak is sampled can be neglected since the total sample thickness is $\sim 10^4$ times the thickness of the MQW structure. Broadening due to the increase in surface temperature, on the other hand, is expected since the FWHM increases with temperature. PL measurements performed on the MQW sample at 30 K for excitation densities 10.3, 16.2, and 23.4 W/cm$^2$ resulted in an increase in FWHM values of 4.2, 3.5, and 2.9 meV, respectively, relative to the values measured at 11 K. According to this, a temperature increase from 11 to 32 K is expected to increase the FWHM of the 1.3 W/cm$^2$ peak by more than 4.2 meV. However, the actual increase in FWHM when increasing the excitation density from 1.3 to 23.4 W/cm$^2$ was only 3.5 meV. This indicates that the actual surface temperature was lower than predicted by the calculations based on the shift in peak position, and that other mechanisms have contributed to the observed behaviour of the PL peak.

For low excitation densities, virtually all electrons (holes) in the conduction (valence) band are assumed to populate states very close to the quantum well ground state. However, increasing the excitation density forces the carriers to populate states of increasingly higher energies, and this both shifts the PL peak toward higher energy and broadens the…
peak. Furthermore, lateral inhomogeneities in the Cd mole fraction are likely to be present, as has been seen for another ternary material system [9]. Carriers will tend to collect in areas with a lower Cd mole fraction in either the well or the barrier layers, and hence a smaller effective bandgap, than the surrounding crystal. When the excitation density increases, more and more carriers are forced to populate states in areas with a higher effective bandgap and the PL peak is shifted to higher energy. Inhomogeneities in the well layers will contribute the most to this effect as the transition energy depends only weakly on the barrier composition.

4. Summary
The PL spectrum of a four-period MQW structure at 11 K was investigated for different excitation densities. It was observed that the peak position was shifted toward higher energy by 2.6 meV and that the FWHM was increased from 7.4 to 10.9 meV when the excitation density was increased from 1.3 to 23.4 W/cm². The FWHM of 7.4 meV is, to our knowledge, the lowest value reported for a CMT MQW structure. The behaviour of the PL peaks is most likely due to a combination of three different mechanisms; heating of the sample by the laser, filling of the quantum well states, and inhomogeneities in the Cd mole fraction.

Acknowledgements
Torgeir Lorentzen and Laila Trosdahl-Iversen are acknowledged for performing the transmission spectroscopy and substrate preparation, respectively. The work was supported by the AFOSR, under grant number FA9550-06-1-0484, P00002.

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