Magnetic origin of the temperature variation of the band offsets in the CdTe/(Cd,Mn)Te heterostructures

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Abstract
Precise temperature dependent measurements of energy of excitons confined in CdTe/CdMnTe quantum wells and superlattices were performed between 2K and 100K. We show that magnetic fluctuations lead to a variation of the valence band offset, in agreement with a model proposed previously for bulk materials.

PACS: 73.20.Dx, 75.50.Pp, 78.66.Hf

1. Introduction

Introduction of semimagnetic (diluted magnetic) semiconductors in the growth of low-dimensional structures allowed to create a wealth of new interesting phenomena related to giant magnetic shifts of energy bands in these compounds [1]. One of the best known materials in this family is cadmium manganese telluride. Band offsets in the CdTe/(Cd,Mn)Te system have been a subject of a prolonged controversy. The difficulty lied in an apparent strong dependence of the relative valence band offset on the Mn mole fraction in the (Cd,Mn)Te barriers of CdTe quantum wells, when studied by measurements of the Zeeman effect of the confined carriers (excitons). The available data ranged from almost zero to about 45% according to the composition and measurement method. The discrepancy has been explained by recognising the strong influence of interfaces on the Zeeman effect experienced by confined carriers. This recognition allowed B. Kuhn-Heinrich et al.[2] to obtain a composition-independent value for the relative valence band offset of about 30% from low-temperature energies of confined hh and lh states. In this work we would like to consider the contribution to the energy gap due to magnetic fluctuations. This contribution was shown [3,4] to be negative and proportional to the product of temperature and magnetic susceptibility. This decrease is distributed between the conduction and the valence bands, proportionally to the product of square of corresponding ion-carrier exchange integral and effective mass. This product has much higher value for the valence band and therefore magnetic fluctuations may influence the band offsets. At low temperatures this contribution is very small, therefore the conclusions from previous works based on low - temperature data remain valid. However, already at 100 K the magnetic contribution may exceed the usual (nonmagnetic) temperature variation of the gap. The objective of this work is to verify whether the temperature variation of the band gap in (Cd,Mn)Te is distributed between the conduction- and the valence bands according to the magnetic fluctuation model, by means of temperature dependent measurements of energies of excitons confined in CdTe/(Cd,Mn)Te heterostructures.

2. Samples and experimental

For our experiments we used structures grown by molecular beam epitaxy (MBE) from CdTe, Te, Cd and Mn sources on (100)-oriented GaAs substrates with CdTe or CdMnTe buffers. The substrate temperature during the growth was approximately 240°C. The manganese mole fraction of the barrier material was chosen high enough to obtain significant contribution of magnetic fluctuations to the temperature variation of energy gap: x=0.375 for sample containing quantum wells and x=1 for superlattices. The well width was chosen not too large to assure a sufficient sensitivity of the exciton energy to the valence band offset but not too small, to obtain very sharp reflectivity structures.

The first sample (CT/CMT 12054A) contained six quantum wells of the thickness 134Å, 66Å, 52Å, 40Å, 27Å and 20Å respectively grown on a CdMnTe buffer. The thickest QW with small exciton confinement energy allowed to measure the energy gap of the well material as a function of temperature.

The second and third samples, (CT/MT 09124 and CT/MT 09074), contained superlattices: 200 periods of CdTe wells separated by MnTe barriers of the thickness 2 and 8 mono-layers respectively. The thickness of wells was 40Å and 45Å respectively.

The precise parameters of all quantum wells were obtained by the Zeeman effect measurements performed at temperature 1.9K and magnetic field up to 5T. Magnetoreflectivity measurements were performed in the Faraday configuration with samples mounted strain-free in a superconducting magnet.

The temperature dependence of the energy gap for MnTe and CdMnTe with high Mn mole fractions was measured for MBE grown layers of thickness above 1μm by magnetoreflectivity [6].

3. Results and Discussion

The low temperature reflectivity spectra, zero-field and in field of 5T, obtained on the typical sample CT/CMT 12054A containing six quantum wells are shown in figure 1. We have identified structures marked by vertical lines, as related to heavy hole ground state excitons in particular quantum wells. Zeeman splittings were used for precise characterisation of the wells. The exciton splittings were described in terms of the model described in [7]. We assumed an intermixing profile between CdTe and CdMnTe represented by an exponential function, with characteristic length l_{int}. Any variation of

the potential in the plane of the interface was neglected. The potential shapes across interfaces were calculated using bulk dependence for local Mn mole fraction. The values of band gap of CdMnTe with high Mn mole fractions were obtained by the magnetoreflectivity measurements [6]. For calculations of the Zeeman effect, the relative valence band offset of 30% was taken. The ground states of electrons and heavy holes were found by numerical integration of the Schrödinger equation as a function of magnetic field. Transition energies were obtained for the two circular polarisations. The intermixing length and well thickness were fitted to the experimental data. The intermixing length was obtained to be between 3.5Å and 4.9Å and indicates quite good quality of interfaces.
The zero-field reflectivity spectra were measured up to 100K. All exciton energies decreases in higher temperatures due to the variation of the energy gap of both CdTe and CdMnTe materials. The exciton energies were calculated using the model developed for Zeeman effect simulations with introduced temperature dependence of energy gaps. To reduce the influence of strain in the sample and insufficient precision of CdTe energy gap temperature variation data, we analysed the differences between the energy of exciton localised in thin quantum wells and exciton localised in the thickest (134Å) one. The results are shown on the figure 2. The calculations were performed in two cases: assuming constant relative valence band offset equal 0.3 or assuming that the difference of energy gap temperature variation between CdMnTe and CdTe, which is due to magnetic fluctuations, originates from the valence band only. The second case means the decrease of the relative valence band offset from 0.3 at 1.9K to 0.237 at 100K for Mn mole fraction in barrier x=0.375. The experimental results clearly favour the second case.
A similar analysis was done for samples CT/MT09124 and CT/MT09074 containing superlattices. The results are presented in figure 3. The experimental points were obtained as a difference between the energy of the exciton in the superlattice and the value of energy gap of the CdTe (well material). The simulations were done in terms of the same model as for quantum wells. The experimental data are much better described by the calculations performed with the assumption of the variation of the valence band offset with temperature. The theoretical curves exhibit a non-linear feature reproducing the energy gap behaviour close to the antiferromagnetic transition of the bulk MnTe [6]. The experimental points do not reproduce this feature. This may be caused by dimensionality dependence of the barrier MnTe magnetic properties.
In summary, our results show that the contribution to the temperature variation of the CdMnTe band gap due to magnetic fluctuations causes a significant change of the relative valence band offset. That effect is observed by the precise measurements of the energies of excitons confined in the quantum wells.
Acknowledgements: This work was in part supported by the KBN grant PBZ-Z011/P4/93/01.

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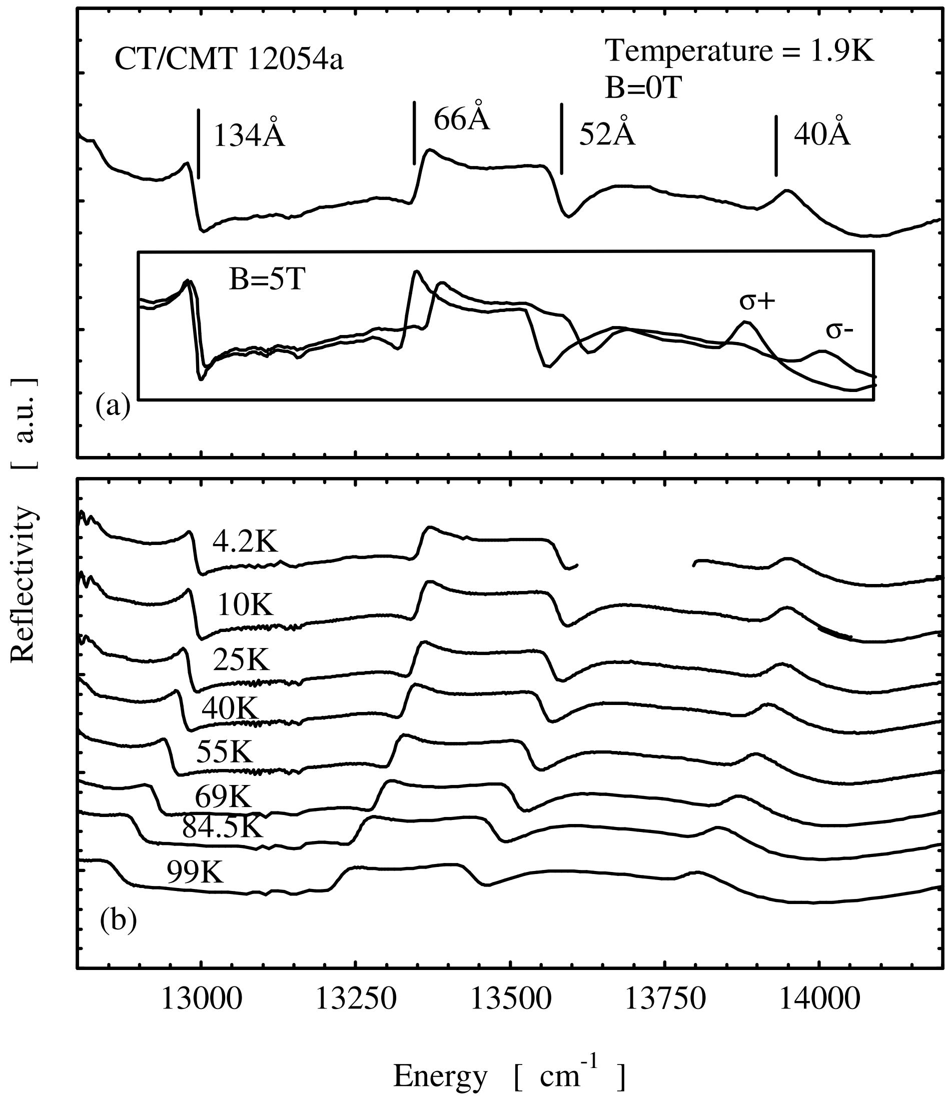
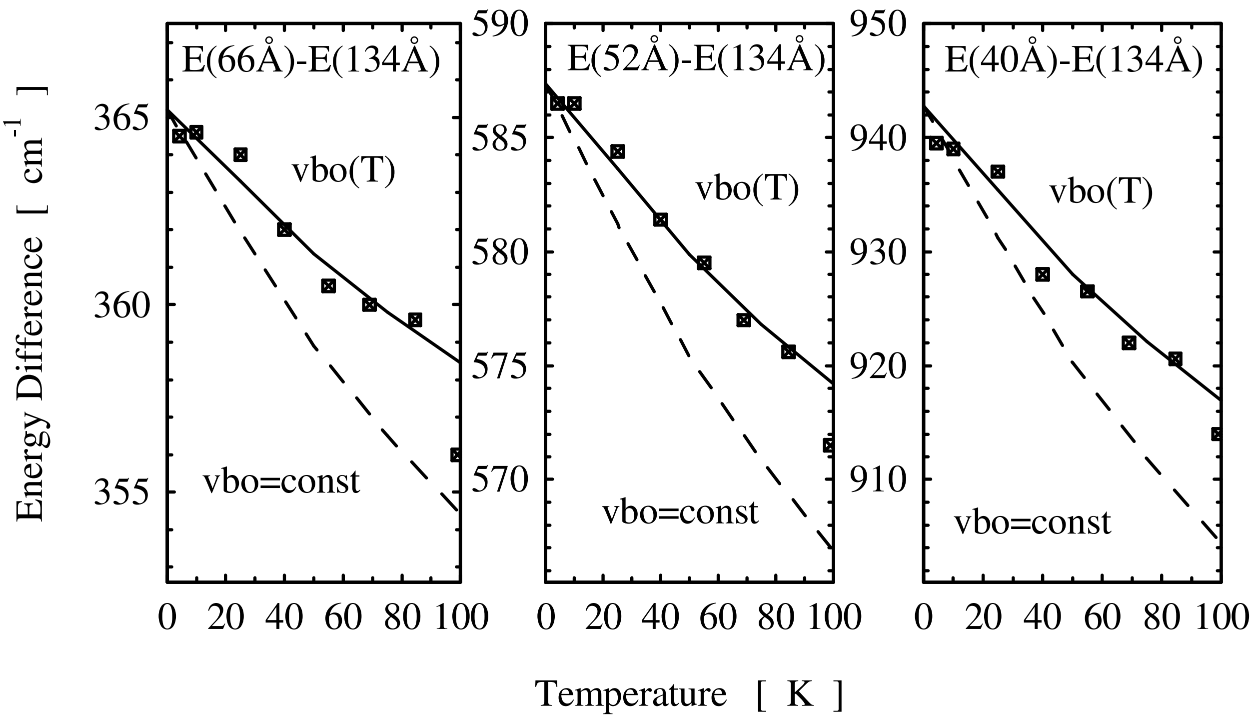
Figure Captions

1. Typical low-temperature magnetoreflectivity spectra (sample 12054a)

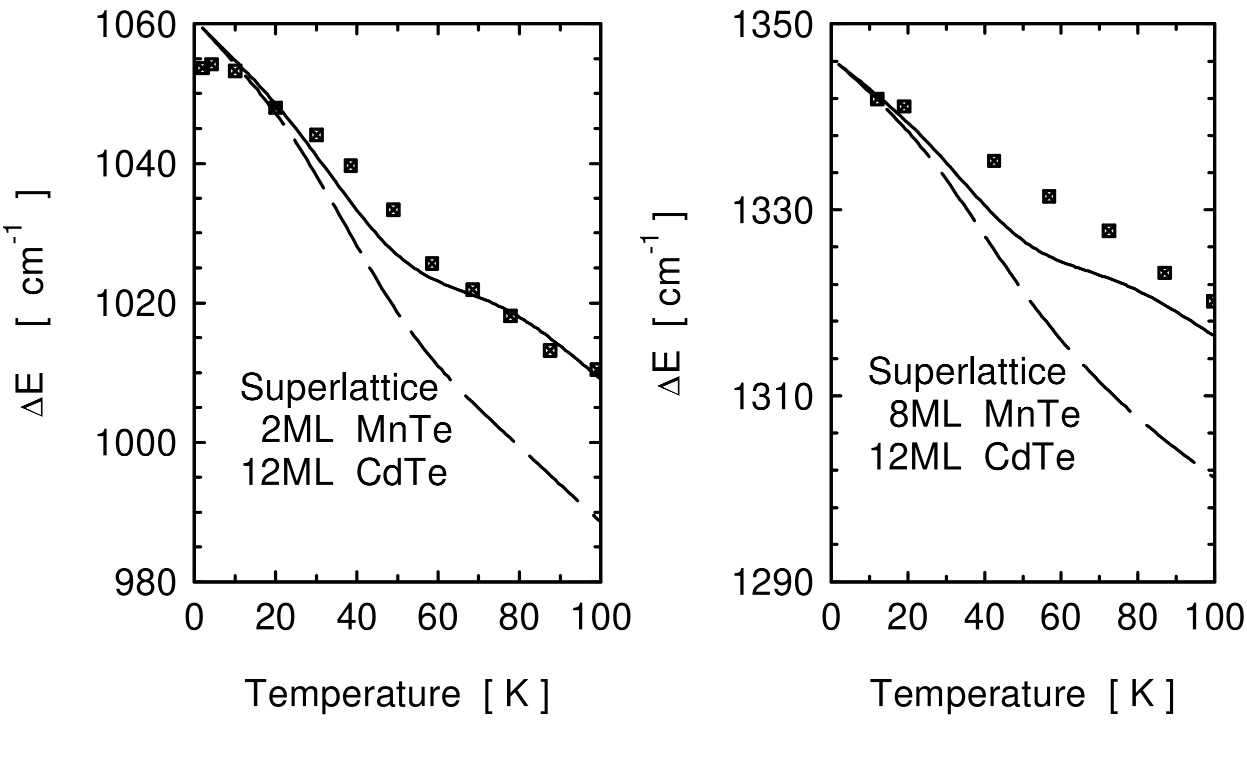
2. Difference between energies of excitons confined in quantum wells of different width vs. temperature. Points represent experimental data, lines-simulations: solid-vbo dependent on temperature, dashed-constant vbo.

3. Difference between superlattice exciton energy and the energy of the CdTe band gap vs. temperature. Points represent experimental data, lines-simulations: solid-vbo dependent on temperature, dashed-constant vbo.


CT/CMT 12054a
Temperature = 1.9K
B=0T
134Å
66Å
52Å
40Å
B=5T
σ+
σ-
(a)
Reflectivity [a.u.]
4.2K
10K
25K
40K
55K
69K
84.5K
99K
(b)
13000
13250
13500
13750
14000
Energy [cm-1]



E(66Å)-E(134Å)
E(52Å)-E(134Å)
E(40Å)-E(134Å)
vbo(T)
vbo=const
Energy Difference [cm^{-1}]
Temperature [K]



Superlattice
2ML MnTe
12ML CdTe
Superlattice
8ML MnTe
12ML CdTe
ΔE [cm^{-1}]
Temperature [K]