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Modification of energy bandgap in lattice mismatched InGaAs/GaAs heterostructures

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This paper addresses some physical aspects and presents experimental results concerning to phenomena which evoke modification of band structure in lattice mismatched InGaAs/GaAs heterostructures, namely the introduction of extra deep-lying energy levels in the bandgap. The deep level transient spectroscopy reveals commonly observed deep level defects in GaAs-based structures associated with native point defects as well as misfit dislocations related to strain relaxation processes.

Keywords: bandgap energy, lattice mismatch, deep level defects, InGaAs heterostructures, deep level transient spectroscopy (DLTS).

1. Introduction

The intrinsic properties of a semiconductor, as reflected by the chemical composition and crystalline structure, can lead to the unique electronic properties of the material. The electronic properties can be changed due to the ability to tailor the band structure, thus novel devices can be conceived and designed for superior and tailorable performance. It is important to establish the physical concepts which are responsible for band structure modifications. There are three widely used approaches in bandgap engineering [1]:

1. Alloying of two or more semiconductors.
2. Use of heterostructure to cause quantum confinement.
3. Use of built-in strain *via* lattice mismatched epitaxy.

The easiest way to alter the electronic properties or to produce a material with new properties is based on making an alloy. The desire to form alloys in semiconductors is motivated by two objectives [1]:

1. Achieving a desired bandgap – this motivation requires a great deal of alloy studies in the laser/detector area. The bandgap essentially determines the energy of the light emitted and absorbed.

2. Creation of a material with a proper lattice constant to match or mismatch an available substrate.

One of the most important reasons of potential applications of semiconductors in electronics and optoelectronics is the possibility of modifying their electronic properties and band structure by incorporation of impurities or other defects. Some of the lattice defects (*e.g.*, impurities, vacancies, interstitials), so-called dopants, are needed for doping the material with shallow donors and acceptors determining the type of majority carriers, their concentration and mobility. The other point defects, so-called deep impurity levels, are associated with the isolated energy levels usually situated deep in the bandgap, and they can determine a lifetime of minority carriers. In contrast to deep point defects, the spatially extended defects (*e.g.*, dislocations, grain boundaries, precipitates) are rather associated with one-dimensional energy bands and they consist of a large number of electronic states [2–4]. Extended defects are known to act as recombination centres or traps for free carriers (thus affecting their concentration, mobility and lifetime) and interact with point defects.

Especially, lattice mismatched heterostructures offer a high flexibility in tailoring their electrical and optical properties, due to the presence of elastic strain. A stable elastic strain changes the bandgap energy, namely it shifts the energy gap between the valence bands and the lowest conduction band, splits the heavy hole and the light hole valence bands, or induces coupling between neighboring bands. Furthermore, it influences the electron (hole) effective mass [5]. Due to the difference in lattice parameters between the epitaxial layer and the substrate, strains can be relieved by generation of so-called misfit dislocations, usually associated with deep energy bands in the bandgap [2–4].

In this paper, we will briefly review some generic and specific properties of lattice mismatched heterostructures and present some of our studies on the electronic structure of the bandgap in the partially relaxed $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{As}/\mathrm{GaAs}$ heterostructures with a small indium content.

2. Deep level defects in InGaAs/GaAs heterostructures

In the relaxation process of lattice mismatched $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{As}/\mathrm{GaAs}$ heterostructures, the elastic strain in the epitaxial layer is relieved by the formation of misfit dislocations at the interface, additionally accompanied by preexisting threading dislocations. Dislocations are known to give rise to the deep-lying, closely spaced energy levels in the bandgap, where the capture and emission processes are controlled by a time dependent barrier hight of the electrostatic Coulombic potential [3]. They form one-dimensional energy bands, which usually act as non-radiative recombination centers or traps for free carriers. Thereby they can significantly affect the density of charge carriers, their mobility and lifetime or interact with point defects by acting as sinks or sources. For these reasons, the ability of controlling defects in these semiconductors is enormously important with respect to designing and manufacturing the high-speed electronic and optoelectronic devices. The investigation, characterization and identification of deep level point and extended defects make it possible to control their influence on device performance and reliability [6].

The deep level transient spectroscopy (DLTS) [7, 8] is currently one of the most powerful and well established diagnostic tools for studying and characterizing deep energy levels associated with point as well as extended defects. It provides many important defect characteristics, such as the energy level position, capture cross-section or defect concentration. The DLTS study of both kinds of defects involves very careful data analysis to separate their specific features emerging from the spectra. Dislocations, due to their many-electron character, add a distinct complexity to the DLTS formalism, like a "logarithmic capture law", *i.e.*, a linear dependence of the DLTS-line amplitude on the logarithm of the filling-pulse time or non-exponential capacitance transients resulting in broadened DLTS-lines. The analysis of DLTS-line shape and behaviour, as well as the measurements of capture kinetics of free charge-carriers by deep level traps, make it possible to distinguish between the point defects and dislocations [3, 4]. Additionally, this enables specification of the type of electronics states at dislocations, namely "bandlike" and "localized" ones [2].

2.1. Experiment

The subject of our investigation were lattice matched GaAs/GaAs and lattice mismatched $In_xGa_{1-x}As$/GaAs heterostructures grown by atmospheric pressure metalorganic vapour-phase epitaxy (AP-MOVPE) system manufactured by AIXTRON. The lattice matched structure consists of 1 μm n-GaAs epitaxial layer grown on (001)-oriented n^+-GaAs substrate doped with Te at about 10^{18} cm^{-3}. The lattice mismatched $In_xGa_{1-x}As$ layers were grown on the same n^+-GaAs substrate, preceded by a 0.5 μm thick n-GaAs buffer layer, doped with Si at about 10^{17} cm^{-3}. All the epitaxial layers differ in indium content x equal to 7.5%, 7.7%, 8.6%, which results in lattice mismatched parameter of about 0.53%, 0.55% and 0.62%, respectively. The aim of the experiment was to obtain partially relaxed epitaxial layers with a small lattice mismatch, less than 1%, in order to offer good conditions for generation of 2D network of 60° misfit dislocations at the interface. The results of structural characterization were published elsewhere [9].

For DLTS experiment, Schottky diodes were made on the front side of the samples and ohmic contacts on their backsides. This enables us to investigate only the majority carriers capture and emission process by deep energy levels. The DLTS system used in our investigations is based on the lock-in type DLS-82E spectrometer (SemiTRAP), equipped with LN_2 bath type cryostat. The other relevant details of the DLTS set-up and samples preparation for electrical characterization are described in [10].

2.2. DLTS results

The DLTS measurements revealed three deep electron traps (labeled E1, E2 and E3) in GaAs/GaAs and two deep traps (EG1 and EG2) in $In_xGa_{1-x}As$/GaAs heterostructures. Exemples of DLTS temperature spectra, obtained for 25 Hz lock-in frequency, are given in Fig. 1.

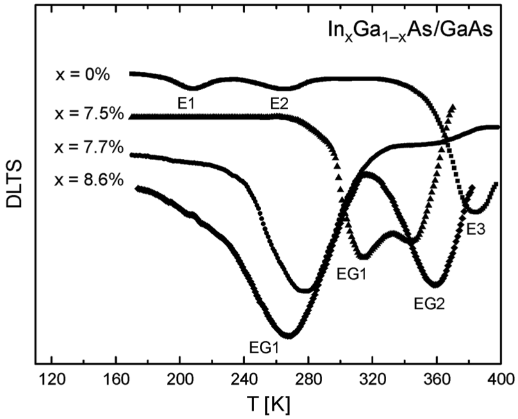

Fig. 1. Representative DLTS temperature spectra of the In$_x$Ga$_{1-x}$As/GaAs heterostructures for different indium contents.

The activation energies, *i.e.*, energy level positions in the bandgap (E_C–E_T) and capture cross-sections (σ_n) have been obtained from the temperature dependence of the thermal emission rates (Arrhenius plots) by means of the standard least-squares fitting procedure (Fig. 2). The calculated parameters of all the electron traps are given in the Table.

Table. Activation energies and capture cross-sections for all the electron traps revealed in GaAs/GaAs and In$_x$Ga$_{1-x}$As/GaAs for different indium content.

Structure	In content	Trap	E_C–E_T [eV]	σ_n [cm^2]	Identification
GaAs/GaAs	$x = 0\%$	E1	0.38	1.1×10^{-14}	EL5 (or EL6)
		E2	0.41	2.6×10^{-16}	EI1 (or EL3)
		E3	0.76	1.5×10^{-14}	EL2
In$_x$Ga$_{1-x}$As/GaAs	$x = 7.5\%$	EG1	0.69	–	ED1
	$x = 7.7\%$	EG1	0.58	–	ED1
	$x = 8.6\%$	EG1	0.43	–	ED1
	$x = 7.5\%$	EG2	0.73	2.1×10^{-14}	EL2
	$x = 8.6\%$	EG2	0.72	4.2×10^{-14}	EL2

The electron traps (E1, E2 and E3) revealed in the GaAs/GaAs have been attributed to the point defects, because they all show a distinct saturation of their DLTS-peak amplitudes versus filling pulse times (see an example relation for E3 trap in the inset of Fig. 2). Such behaviour, called the "exponential capture law", is characteristic of the point defects. A careful analysis of the obtained parameters enables us to identify the traps E1 as As-antisite–As-vacancy complex (As$_{\mathrm{Ga}}$–V$_{\mathrm{As}}$) related level EL6 [11] or divacancy complex (V$_{\mathrm{Ga}}$–V$_{\mathrm{As}}$) related level EL5 [12], E2 as oxygen associated levels EI1 or EL3 [13, 14]. Furthermore, the trap E3 was identified as a well-known deep

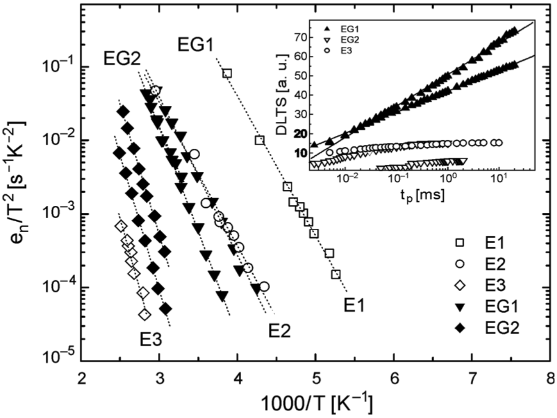

Fig. 2. Arrhenius plots for the electron traps revealed in the GaAs/GaAs and $In_xGa_{1-x}As$/GaAs heterostructures. The dotted lines represent the best least-squares fit to the experimental data. The inset shows amplitudes of the DLTS peaks of the traps as functions of the filling-pulse duration.

level EL2, which is mainly due to As-antisite defect (As_{Ga}) being a dominant native point defect in GaAs-based structures [15]. A similar exponential capture kinetics was also observed in the case of the trap EG2 revealed in $In_xGa_{1-x}As$/GaAs heterostructures. Moreover, its parameters are also very close to that of EL2 level.

On the contrary, the trap EG1, observed in all the $In_xGa_{1-x}As$/GaAs ternary compound heterostructures reveals no saturation up to the longest filling pulse times, used in the experiment (inset of Fig. 2). A linear dependence of the DLTS-peak amplitude on the logarithm of the filling pulse duration, generally called the “logarithmic capture law”, is the characteristic feature of spatially extended, many electron defects, *e.g.*, dislocations [16]. They form deep-lying closely-spaced energy levels, forming a dislocation band, which can be hardly fill with free charge carriers due to the time-dependent Coulombic barrier of the repulsive electrostatic potential built up upon the defect. This barrier limits the successive capture of the carriers during the filling process. This phenomenon is considered as a principal argument for distinguishing between point defects and dislocations [3, 17].

From the Arrhenius plots (Fig. 2), we obtained different activation energies of the trap EG1, which generally decrease with increasing indium content in the epitaxial layer. Moreover, it scales linearly with the change of the bandgap energy due to the various composition, *i.e.*, the trap EG1 represents a constant position of its energy level with respect to the top of the valence band, equal to about 0.74 eV [10]. A similar dependence occurs in the case of the well-known electron trap ED1, observed in many lattice mismatched $A^{III}B^{V}$ heterostructures and generally associated with the electronic core states at misfit or threading dislocations [18, 19]. Due to the anisotropic relaxation of a misfit strain, the asymmetric 2D network of 60° misfit dislocations has been generated at the interface of the $In_xGa_{1-x}As$/GaAs heterostructures under investigation [9]. As the maximum of the depth concentration profile for the trap EG1 was

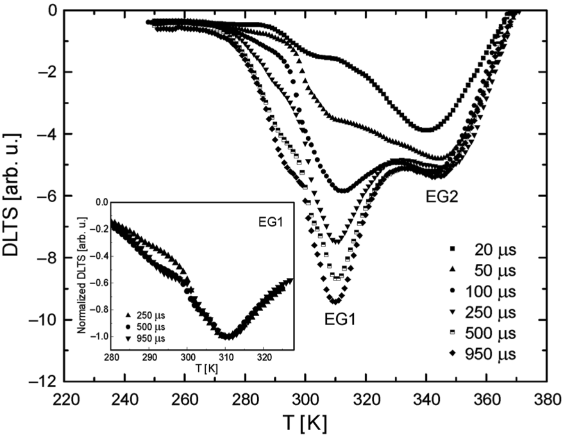

Fig. 3. Exemples of DLTS temperature spectra of the lattice mismatch $In_{0.075}Ga_{0.925}As/GaAs$ heterostructure for different filling pulse times. The inset shows a normalized plot of the DLTS-line amplitude of the dislocation related deep electron trap EG1.

localized near the interface between the layer and the substrate [10], we concluded that the trap could be attributed to the electronic states at misfit dislocations. The results obtained enable us to identify the trap EG1 as the ED1 one.

Furthermore, in the framework of the so-called barrier model of extended defects [2], the electronic states at dislocations can be classified as "localized" or "bandlike" using DLTS technique. In this model, both types of states can be distinguished by the variation of the DLTS-line amplitude of the dislocation-related deep level defect on the filling pulse time. For the "localized" states, the DLTS-line maximum stays generally constant and its high temperature sides coincide after normalizing, while in the case of the "bandlike" states the DLTS-line maximum shifts towards lower temperatures with simultaneous coincidence of its high temperature sides [2].

According to this model, we did not observe any distinct shift of the maximum of the EG1 peak amplitude for all the $In_xGa_{1-x}As/GaAs$ heterostructures, as shown in Fig. 3 (see also Ref. [10]) for the structure with 7.5% indium content. Moreover, after normalizing its high temperature sides match each other (see the inset of Fig. 3). Finally, these findings enable us to attribute the EG1 trap to the "localized" states at misfit dislocations.

3. Conclusions

In the paper, some inevitable phenomena modifying a structure of the energy bandgap in lattice mismatched $In_xGa_{1-x}As/GaAs$ heterostructures, both pseudomorphic and partially relaxed have been presented. The DLTS technique makes it possible to reveal several deep energy levels in the bandgap, associated both with point and extended defects. All the deep levels have been distinguished and identified on the basis of their parameters and a DLTS-line shape and behaviour analysis. Especially, a thorough analysis of the DLTS-data connected with the electron trap EG1, enabled us to attribute this trap to ”localized” states at misfit dislocations, lying at the interface between the epitaxial layer and the substrate of partially relaxed samples. The other traps were ascribed to point defects or defect complexes.

Concluding, the built-in elastic strain considerably affects the band structure as well as offers the additional flexibility to modify and tailor the electronic structure and optical response of the epitaxial layer. Many electronic and optoelectronic devices have benefited from such band structure modifications. Unfortunately, a strain relaxation process leads to a significant degradation of the layer quality and it intorduces extra dislocation-related deep energy levels in a bandgap region. Most of the deep levels act as trap centers, thus they strongly influence the functional availability of devices. Therefore, detection and control of the deep level defects are strongly connected with the improvement of the device technology and their properties.

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