Quality diagnostics of nanoscale AlAs/GaAs resonant tunnelling heterostructures based on IR-spectroscopic ellipsometry

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Abstract. In this work, the procedure of assessing the quality of AlAs/GaAs resonant tunnelling heterostructures with relation to their resistance to diffusion destruction was developed. The diffusion blur of the AlAs/GaAs heterostructure layers was detected by means of infrared-spectroscopic ellipsometry. The diffusion coefficients of Al and Si in GaAs were also calculated.

1. Introduction

The use of semiconductor devices based on the quantum size effects of charge transport is one possible means of improving the quality of radio electronic systems. Such devices are resonant tunnelling diodes (RTD) based on multilayer nanoscale AlAs/GaAs resonant tunnelling heterostructures with transverse charge transport. The short tunnelling time of the electrons provides extremely high performance of the diode (frequency up to 1 THz) and suppression of the shot noise [1].

By varying the parameters of the heterostructure layers (thickness, elemental composition), one can vary the I-V curve shape. Such properties of RTD allow one to create different nonlinear radio signal converters, including mixers, rectifiers, multipliers, and SHF and EHF generators [2-3]. There is an extensive bibliography devoted to studying RTD properties and issues with their technical radio applications, but the reliability of such devices requires further investigation. The problem of a reliability study of RTD is being solved by kinetics analysis of physical degradation processes in the RTD structure.

An RTD consists of a resonant tunnelling structure (RTS) (set of layers of AlAs/GaAs), contact regions (layers of Si-doped GaAs), and ohmic contacts. RTD I-V curve is highly sensitive to the changes of RTS parameters because RTS layers are very thin: only up to a few nanometers. Degradation processes (interlayer diffusion of Al in RTS and Si in contact regions) lead to changes in the shape of the potential barrier and potential well and, therefore, to changes of charge transport conditions in the structure (figure 1). Diffusion blur of ohmic contacts leads to an increase in their contact resistance. In turn, these processes lead to 'rifting' of the RTD I-V curve and deterioration of the output electrical characteristics of radio signal converters based on RTD.

The aim of the present work is the development of a technique allowing one to identify the diffusion coefficients of Al and Si in GaAs and to carry out quality diagnostics of resonant tunnelling heterostructures (RTHS) in relation to their resistance to diffusion destruction. Knowledge of the kinetics of diffusion processes in an RTD structure will allow one to predict reliability against gradual failures of RTDs and nonlinear radio signal converters.

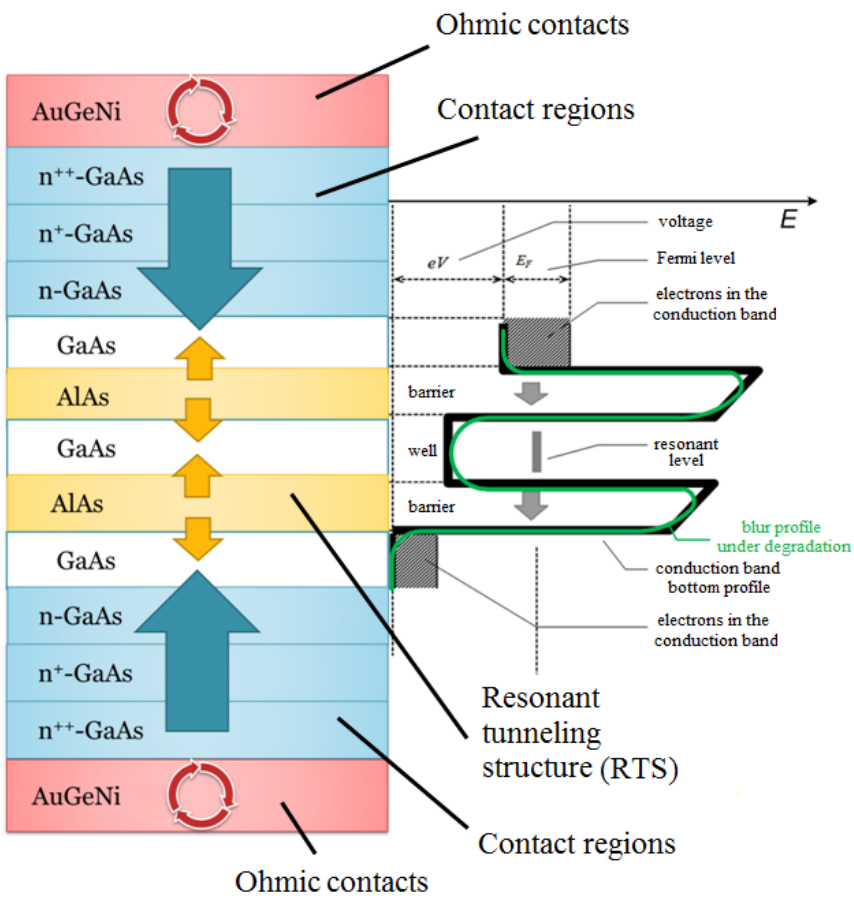

Figure 1. Structure and possible degradation phenomena. Yellow arrows: aluminium diffusion, blue arrows: silicon diffusion, circular red arrows: diffusion in ohmic contacts.

2. Results

The degradation of AlAs/GaAs RTHS as a result of Al diffusion in RTS and Si diffusion in the contact regions is considered. The intensity of diffusion processes in AlAs/GaAs RTHS is characterised by the diffusion coefficients of Al and Si in GaAs. Accordingly, quality assessment of RTHS (with relation to the resistance to diffusion destruction) is carried out based on the values of the diffusion coefficients of Al and Si in GaAs.

According to references [4-12], the diffusion coefficients of Al and Si in GaAs vary greatly depending on the conditions under which the heterostructures are produced by the means of molecular beam epitaxy (MBE). It is connected by the dependence of defectiveness of the growing heterostructures with respect to numerous technological factors such as substrate temperature (600–650 ºC) during MBE, pressure in the chamber, temperature and time of annealing, defectiveness of the initial substrate, and many more.

The main diffusion mechanism for both Al and Si in GaAs is diffusion via vacancies of gallium (V_{Ga}). This is because atoms of Al and Si have similar masses and sizes and can be arranged in a Ga sublattice (with doping levels less than $5 \cdot 10^{18}$ cm^{-3}). Herein, diffusion occurs predominantly via negatively ionized vacancies of gallium with charge state ‘-3’. The diffusion coefficient depends also on the concentration of n-dopant according to the effect of Fermi level [4-8, 13-14].

The technique of nanoscale AlAs/GaAs RTHS diagnosis was developed for evaluation of diffusion coefficients. Structurally, it consists of the following main stages (figure 2): measurement of ellipsometric parameters of nanoscale AlAs/GaAs RTHS by the means of infrared-spectroscopic ellipsometry (IR-SE) before and after thermal influence, ellipsometric model creation, determination of profile distribution of Si in resonant tunnelling heterostructures, and calculation of diffusion coefficients on the basis of the determined profile.

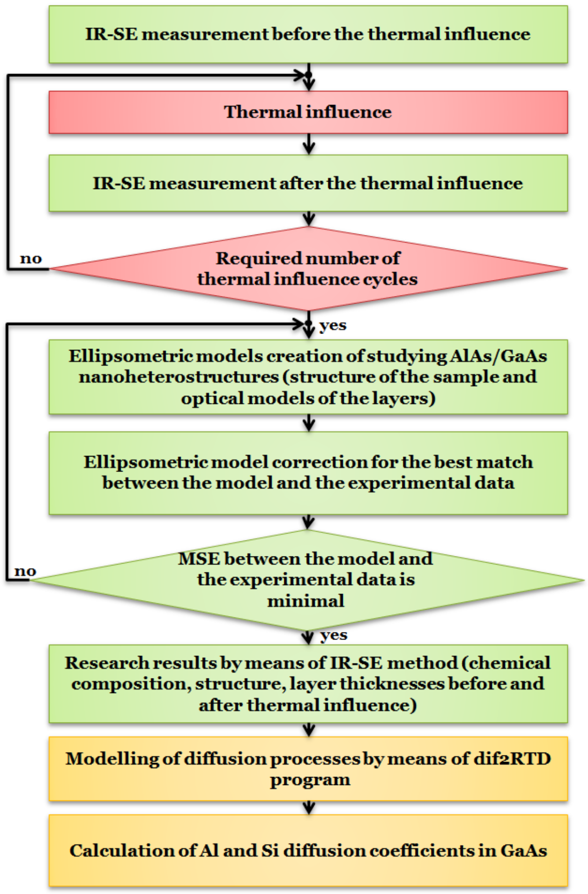

Figure 2. Block diagram of the quality diagnostics technique for nanoscale AlAs/GaAs resonant tunnelling heterostructures based on IR-spectroscopic ellipsometry.

The IR-spectroscopic ellipsometry technique is widely used for determination of thin film thicknesses and optical properties [15-18], semiconductor heterostructures [19-20], changes in chemical composition as the result of modification [21-22], etc.

Ellipsometric studies consist of the following stages: obtaining experimental data (spectra of Ψ and Δ), ellipsometric model creation (optical constants and layer thicknesses), and correction of model parameters for the purpose of obtaining the best fitting of experimental and generated data on the basis of this model obtaining the required results from the studies.

An ellipsometric model of the AlAs/GaAs RTHS samples includes the structure of the sample, optical constants, and thicknesses of all layers. The model is specified during research. Based on the specified ellipsometric model, one can estimate the chemical composition, structure, and layer thicknesses of AlAs/GaAs RTHS before and after thermal influence.

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The calculation of the diffusion coefficients of Al and Si is carried out by the means of the dif2RTD program [23] for modelling diffusion processes in the nanoscale AlAs/GaAs RTHS and the I-V curve of RTD.

Temperature, time, and the number of thermal influences (artificial aging) and the number of measurements on the IR-spectroscopic ellipsometer are determined on the basis of prior data of chemical composition from studying nanoscale A_3B_5 heterostructure and the diffusion coefficients of the RTD heterostructure elements.

Validation of the quality diagnostics technique with regard to nanoscale AlAs/GaAs resonant tunnelling heterostructures based on IR-SE was carried out on two nanoscale heterostructures distinguished by layer structure and substrate temperature during epitaxial growth:

- GaAs (20 nm) / n-GaAs ($n_{Si} = 2 \cdot 10^{17}$ cm^{-3}, 100 nm) / GaAs (300 nm) / GaAs (substrate 450 μm) – Heterostructure № 1 (MBE temperature 650 °C);
- n-GaAs ($n_{Si} = 5 \cdot 10^{18}$ cm^{-3}, 100 nm) / n-GaAs ($n_{Si} = 2 \cdot 10^{17}$ cm^{-3}, 30 nm) / GaAs (1,5 nm) / AlAs (1,7 nm) / GaAs (4,5 nm) / AlAs (3,0 nm) / GaAs (10,0 nm) / n-GaAs ($n_{Si} = 2 \cdot 10^{17}$ cm^{-3}, 30 nm) / n-GaAs ($n_{Si} = 5 \cdot 10^{18}$ cm^{-3}, 100 nm) / GaAs (substrate 450 μm) – Heterostructure № 2 (MBE temperature 600 °C).

Thermal influence on heterostructure № 1 was carried out at a temperature of 530 °C and pressure p = 10^{-4} Pa for 2 hours. Heterostructure № 2 was heated at a temperature of 300 °C for 4, 6, 8, and 10 hours (total annealing time was 28 hours) in the air environment.

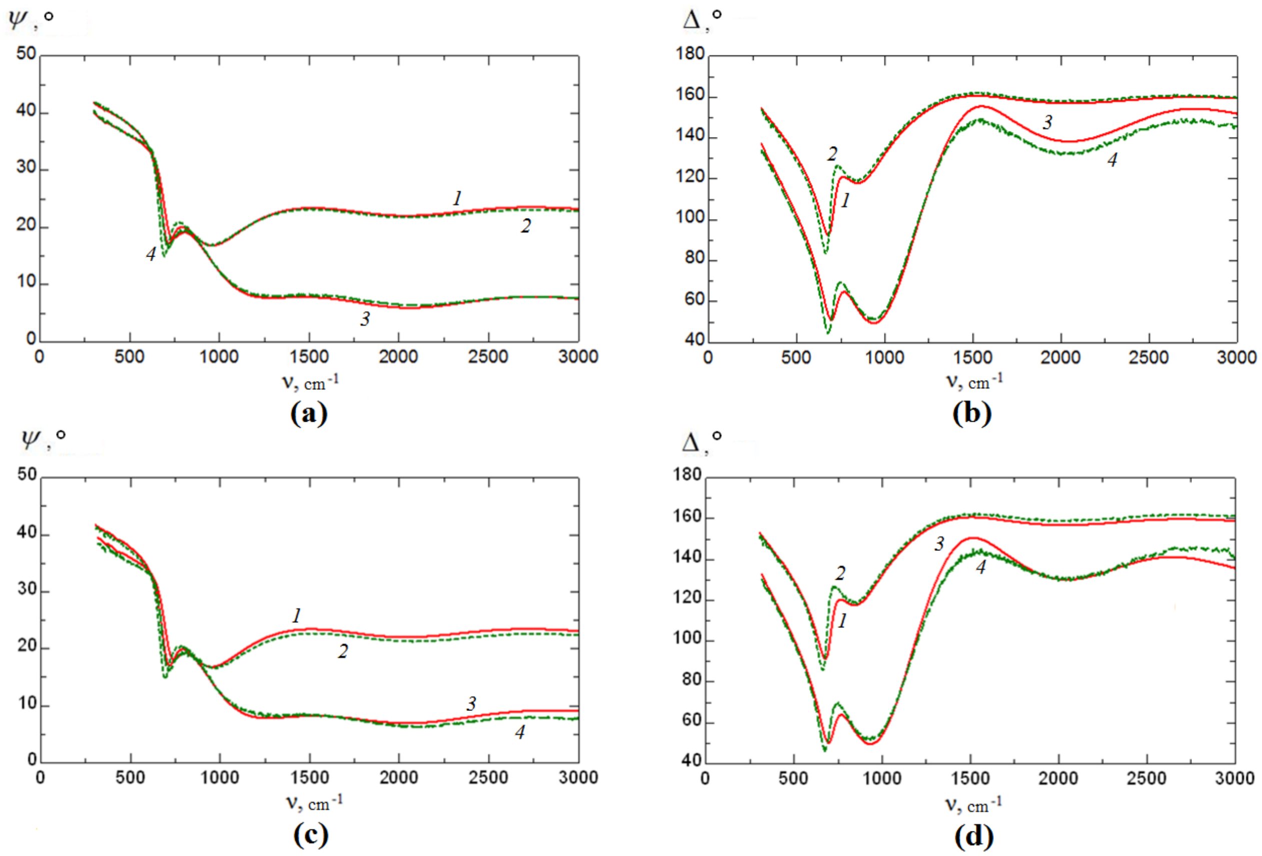

Figure 3. The spectra of the ellipsometric parameters *Ψ* (a, c) and *Δ* (b, d) of the AlAs/GaAs RTHS before (a, b) and after 28 hours (c, d) of thermal influence (*1* – generated data, the angle of incidence equals 60°; *2* – experimental data, the angle of incidence equals 60°; *3* – generated data, the angle of incidence equals 70°; *4* – experimental data, the angle of incidence equals 70°).

Ellipsometric model creation of the studied heterostructures, together with analysis of identified changes of the ellipsometric parameters *Ψ* and *Δ* before and after thermal influence (figure 3), allowed for the identification of diffusion blur of the layers belonging to the heterostructure (figure 4).

On this basis, diffusion coefficients of Al and Si in GaAs in heterostructure № 1 were calculated [20]:

$$D_{Al,Si} = 0{,}17 \cdot \exp\left(-\frac{3{,}5}{kT}\right) \cdot \left(\frac{n_{Si}}{n_i}\right)^3 \tag{1}$$

where $D_{\text{Al,Si}}$ = diffusion coefficients of Al and Si in GaAs,

k = Boltzmann constant (k = 8,617 · 10^{-5} eV·K^{-1}),

T = temperature, K,

n_{Si} = dopant carrier concentration (Si), cm^{-3},

n_i = intrinsic carrier concentration, cm^{-3}.

For heterostructure № 2 [21]:

$$D_{Al,Si} = 0{,}22 \cdot \exp\left(-\frac{3{,}5}{kT}\right) \cdot \left(\frac{n_{Si}}{n_i}\right)^3 \tag{2}$$

Top rough layer	24,9 ± 2,0 nm
n-GaAs heavily Si-doped (5 · 10^{18} cm^{-3})	100,3 ± 1,7 nm
Gradient layer	0 nm
n-GaAs Si-doped (2 · 10^{17} cm^{-3})	30,0 nm
Gallium arsenide GaAs (spacer)	1,5 nm
Aluminum arsenide AlAs (barrier)	1,7 nm
Gallium arsenide GaAs (well)	4,5 nm
Aluminum arsenide AlAs (barrier)	3,0 nm
Gallium arsenide GaAs (spacer)	10,0 nm
n-GaAs Si-doped (2 · 10^{17} cm^{-3})	30,0 nm
Gradient layer	0 nm
n-GaAs heavily Si-doped (5 · 10^{18} cm^{-3})	1005,0 ± 3,0 nm
Gradient layer	0 nm
Substrate GaAs	0,35 mm
Bottom rough layer	90,5 ± 10,0 nm

(a)

Top rough layer	15,9 ± 2,1 nm
n-GaAs heavily Si-doped (5 · 10^{18} cm^{-3})	103,4 ± 1,6 nm
Gradient layer	6,7 ± 1,5 nm
n-GaAs Si-doped (2 · 10^{17} cm^{-3})	30,0 nm
Gallium arsenide GaAs (spacer)	1,5 nm
Aluminum arsenide AlAs (barrier)	1,7 nm
Gallium arsenide GaAs (well)	4,5 nm
Aluminum arsenide AlAs (barrier)	3,0 nm
Gallium arsenide GaAs (spacer)	10,0 nm
n-GaAs Si-doped (2 · 10^{17} cm^{-3})	30,0 nm
Gradient layer	6,9 ± 1,8 nm
n-GaAs heavily Si-doped (5 · 10^{18} cm^{-3})	991,2 ± 3,6 nm
Gradient layer	7,1 ± 1,9 nm
Substrate GaAs	0,35 mm
Bottom rough layer	74,9 ± 10,0 nm

(b)

Figure 4. Ellipsometric models of the RTHS before (a) and after 28 hours (b) of thermal influence.

The pre-exponential factors in (1) and (2) differ by 30 %. Since the diffusion coefficients of Al and Si in GaAs are proportional to the amount of gallium vacancies [13-14, 24], one can conclude that the amount of defect in the studied heterostructures also differs by 30 %. It indicates that technological parameters (in this case MBE temperature) influence production quality (in the sense of the diffusion destruction processes rate) of RTHS. Thus, the IR-SE technique detects differences in the production quality of RTHS at different growing temperatures, and one can apply it for quality control.

3. Conclusions

The production quality of the AlAs/GaAs heterostructure of RTD was assessed in terms of the diffusion coefficient values of Al and Si in GaAs, representing the intensity of diffusion processes in the resonant tunnelling heterostructure.

In the present work, the possibility of using the IR-spectroscopic ellipsometry technique for calculation of the diffusion coefficients of Al and Si in AlAs/GaAs resonant tunnelling heterostructures was shown. Numerical characteristics of degradation processes, obtained in this work, can be used to predict the reliability of RTD and technical radio devices.

This technique developed on the basis of IR-spectroscopic ellipsometry allows one to 'see' the diffusion of the resonant tunnelling heterostructure AlAs/GaAs elements in nanometer layers. It allows one to determine diffusion coefficients of heterostructure elements. Since a diffusion coefficient directly depends on the defect amount in a heterostructure, one can assess the quality of more complex heterostructures and the value of their diffusion destruction in production process and in operation.

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