Optimization of the off-oriented Ge substrates for MOVPE grown GaAs solar cells

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ABSTRACT: GaAs/Ge heterostructures having abrupt interfaces were grown on 2^o, 6^o, and 9^o off-cut Ge substrates and investigated by cross-sectional high-resolution transmission electron microscopy (HRTEM), scanning electron microscopy, photoluminescence spectroscopy and electrochemical capacitance voltage (ECV) profiler. The GaAs films were grown on off-oriented Ge substrates with growth temperature in the range of 600-700^{o}C, growth rate of 3-12 μm/hr and a V/III ratio of 29-88. The lattice indexing of HRTEM exhibits an excellent lattice line matching between GaAs and Ge substrate. The PL spectra from GaAs layer on 6^o off-cut Ge substrate shows the higher excitonic peak compared with 2^o and 9^o off-cut Ge substrates. In addition, the luminescence intensity from the GaAs solar cell grown on 6^o off-cut is higher than on 9^o off-cut Ge substrates and signifies the potential use of 6^o off-cut Ge substrate in the GaAs solar cells industry. The ECV profiling shows an abrupt film/substrate interface as well as between various layers of the solar cell structures.

1. INTRODUCTION

GaAs/Ge heterostructures (HSs) have received a great attention as starting materials for the fabrication of space quality solar cells [1-5]. Although the low lattice mismatch (0.07%) of the GaAs/Ge system suggests nearly dislocation free interface, however, polar-on-nonpolar heteroepitaxy poses several unique problems; like misfit dislocations at the interface, antiphase domains (APDs) in the polar materials, and the cross diffusion of Ga, As and Ge at the GaAs/Ge heterointerface. The APDs separated by antiphase boundaries (APBs) in the III-V compound semiconductors are harmful for devices, which are based on the heterointerface properties, because the APBs act as nonradiative recombination centers [6, 7]. Therefore, the careful control of the substrate surface structure and the initial growth conditions [8-11], like the initial growth temperature, growth rate and the V/III ratio are essential to grow device quality single-domain GaAs/Ge heterostructures. In the present work, we have investigated the effect of off-orientation on metal-organic vapor-phase epitaxy (MOVPE) grown Si-doped n-type GaAs on Ge substrates for solar cell application. The study leads to establish the optimum Ge substrate for the high efficiency solar cell application.

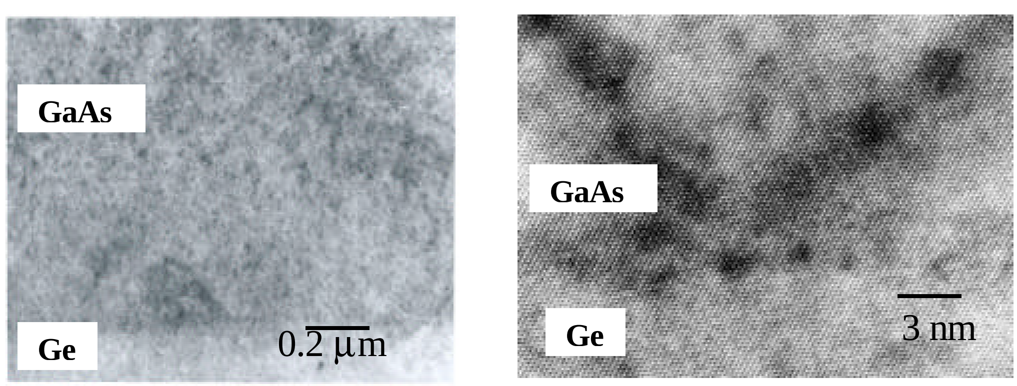
2. EXPERIMENTAL

Si-doped n-type GaAs films and solar cells structures were grown in a low-pressure horizontal MOVPE reactor on Sb-doped n^+- Ge (100) 2^o, 6^o and 9^o off-oriented towards [110] direction. The source materials were TMGa, 100% AsH_3, TMAl, DMZn as a p-type dopant, 104 ppm SiH_4 as an n-type dopant and palladium purified H_2 as a carrier gas. The details of the growth procedure can be found elsewhere [12-14]. The epitaxial GaAs/Ge heterointerfaces were prepared by Ar^+ ion thinning for cross-sectional observations. The HRTEM investigations were performed using a Hitachi H-9000 UHR ultra-high resolution electron microscope operated at 300 kV. The cross-sectional image of the GaAs solar cell structure was determined by scanning electron microscopy. PL measurements were carried out using a MIDAC Fourier Transform PL (FTPL) system at a temperature of 4.2 K and 100 mW laser power. Argon ion laser operating at a wavelength of $5145A^o$ was used as a source of excitation. The exposed area was about 3 mm^2. PL signal was detected by a LN_2 cooled Ge-photodetector whose operating range is about 0.75-1.9 eV. The doping concentrations were determined using an ECV profiler.

3. RESULTS AND DISCUSSION

3.1 Cross-sectional TEM investigation of GaAs/Ge heterointerface

The epitaxial films were investigated by TEM to reveal the characteristics of MDs and other crystalline defect. Figure 1 (a) shows the cross-sectional TEM image of GaAs on 6^o off-cut Ge substrate using an As prelayer with the growth temperature of 675^oC, V/III ratio of 88.20 and a growth rate of 3 μm/hr. It was found that for the layer grown under these growth conditions, the interface between the GaAs epilayer and the Ge substrate is sharp and almost no APDs were observed at the heterointerface. The epitaxial growth of GaAs and Ge substrate is clearly visible in this high-resolution image with the well-resolved GaAs lattice lines extending all the way down to the Ge surface closely matching with the Ge lattice (Fig. 1b).



(a) **(b)**

Fig. 1 [110] cross-sectional high-resolution TEM image of heterointerface of GaAs/(100) Ge 6^o heterostructure.

3.2 Electrochemical capacitance-voltage profile of GaAs/Ge heterostructure

The ECV profiler was used to determine the concentration along depth in the Si-doped GaAs on different off-oriented Ge substrates. Fig. 2 shows one of the ECV carrier concentration profiles of Si-doped GaAs on Ge substrates of 2°, 6° and 9° off-orientation. The GaAs/Ge heterointerface for 6° off-orientation is found to be abrupt as compared with other off-orientations in the same growth conditions. It can be also noticed that there is no p-n junction formed due to simultaneous indiffusion of Ga and As into Ge in all of the off-cut Ge substrates. The carrier concentration is uniform along the depth in 6° Ge substrate and a clear film/substrate interface was observed in all the present investigated films.

3.3 Effect of growth temperature on carrier concentration

The variation in electron concentration has been observed as the growth temperature increased, as shown in Fig. 3 for a fixed SiH_4 mole fraction. The strong temperature dependence of Si incorporation is believed to be a result of increasing decomposition rate of SiH_4 with increasing temperature. The doping incorporation efficiency in GaAs on different off-oriented Ge substrate was almost the same. However, the higher activation energy of Si determined from the slope of this figure is still under investigation.

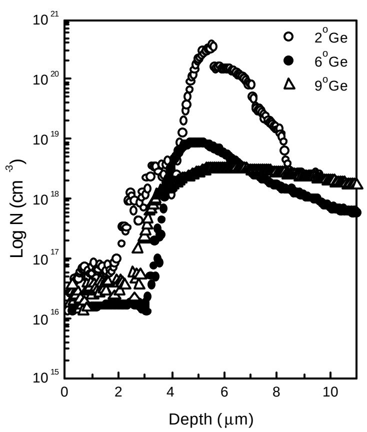


Fig. 2 ECV profile of Si-doped GaAs on 2°, 6° and 9° off-cut Ge substrates. Growth parameters are: 675°C, V/III = 88, 3 μm/hr.

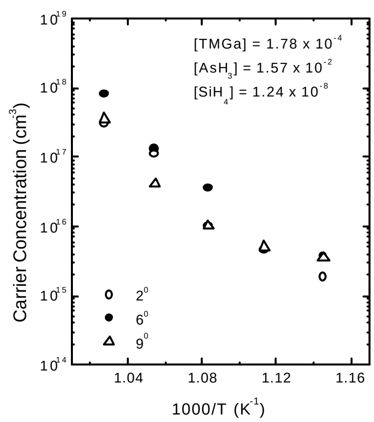


Fig. 3 Electron concentration vs growth temperature on 2°, 6° and 9° off-cut Ge substrates.

3.4 Cross-sectional image of the GaAs/Ge solar cell structure

Fig. 4 shows one of the cross-sectional SEM images of p/n GaAs/Ge solar cell structure. The interface of each layer is also indicated in this figure. Defects are not visible at the GaAs/Ge interface due to the low magnification. These solar cells were grown after optimizing the GaAs layer on different off-oriented Ge substrates.

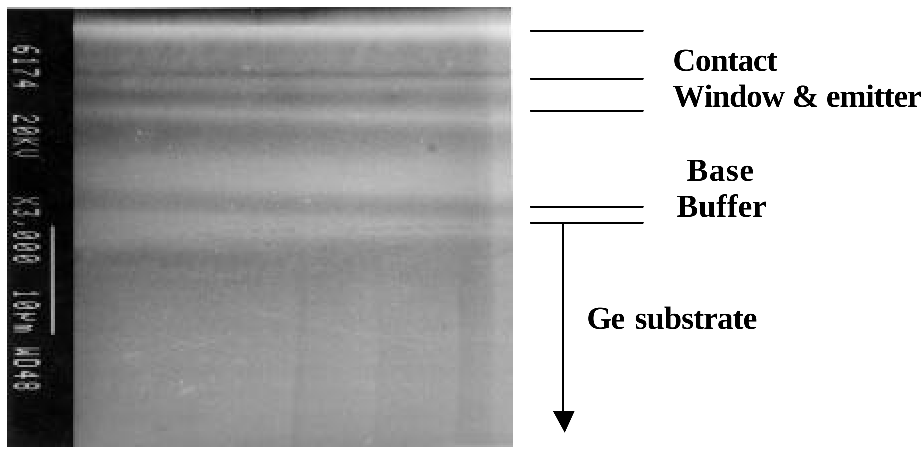


Fig. 4 Cross-sectional SEM image of GaAs/Ge solar cell

3.5 Optical properties on different off-oriented Ge substrates

Fig. 5 shows the PL spectra obtained from the Si-doped GaAs epilayers on 2^o, 6^o and 9^o off-oriented Ge substrates grown at a substrate temperature of 675 ^oC. The Si doping broadens the excitonic emission until it becomes a wide band-to-band (B-B) luminescence. The peak at around 1.49 eV has been attributed to band-to-acceptor (B-A) transitions involving residual carbon (C) impurities present in MOVPE GaAs [15]. The B-A transitions were observed from all the films grown on Ge substrates and the peak intensity due to C decreases with increasing growth temperatures compared with the excitonic peak intensity. The peak intensity due to excitonic transition is higher than C-related transitions on 6^o and 9^o off-oriented Ge substrates, whereas on 2^o off-oriented Ge substrate, the intensities of the two peaks are almost same. Therefore, the 6^o or 9^o Ge substrate would be the proper choice for solar cell growth.

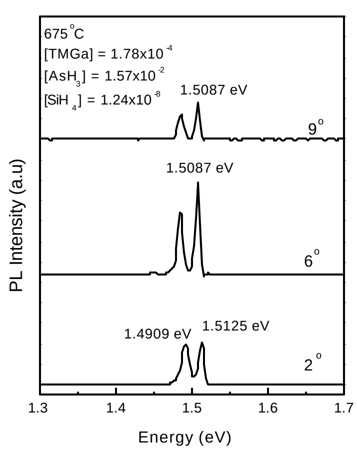


Fig.5 4.2 K PL spectra of Si-doped GaAs epilayers grown on 2^o, 6^o and 9^o off-cut Ge substrates.

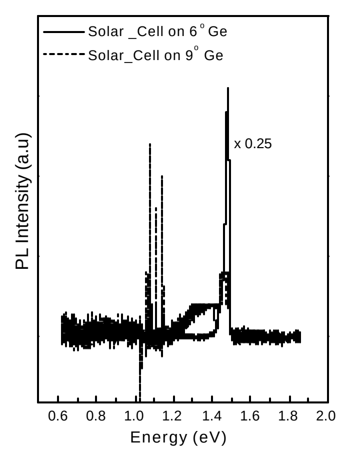


Fig.6 4.2 K PL spectra of GaAs solar cell grown on 6^o and 9^o off-cut Ge substrates.

3.6 Optical characteristics of solar cells

Fig. 6 shows the experimental PL spectra of p/n junction GaAs solar cells grown on 6^o and 9^o structures, measured at 4.2 K. The luminescence efficiency from GaAs/Ge solar cell grown on 9^o off-oriented Ge substrate is very low as compared to the luminescence efficiency from GaAs/Ge solar cell grown on 6^o off-oriented Ge substrates. From this observation one can rule out the possibility of growing solar cells on 9^o off-oriented Ge substrates. Therefore, the selection of the 6^o off-oriented Ge substrate for the GaAs/Ge heterostructure solar cells is justified from the photoluminescence spectroscopy.

3.7 Electrochemical capacitance-voltage profiles of GaAs/Ge solar cell structure

To gain a fundamental understanding of the performance of multi-layered GaAs/Ge solar cell, ECV profiling was used to examine the depth profile of the carrier concentration in each layer, thickness of each layer, and the abruptness between two layers. Fig. 7 shows a typical ECV profile of p/n junction GaAs/Ge 6^o solar cell with controlled interfaces between the two adjacent layers. One can carefully control the MOVPE growth parameters for obtaining a highly abrupt interface between the emitter and base layer of the GaAs/Ge solar cell. During the growth of complete solar cell structure, we had increased or decreased the n-type and p-type dopants input mole fractions depending on the carrier concentration requirement in each layer. Furthermore, the duration of each layer was adjusted prior to the growth rate knowledge of each dopant. We did not profile the carrier concentration inside the Ge substrate since we have seen from Fig. 2 that As concentration can diffuse inside the Ge substrate up to 8-10 µm depending on the growth temperature for the compete solar cell structure.

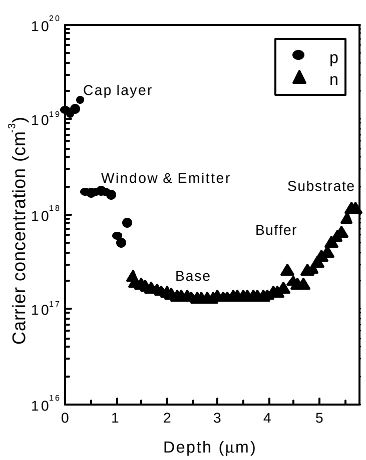


Fig. 7 ECV profile of GaAs/Ge6^o heterostructure solar cell.

4. CONCLUSIONS

The Si-doped GaAs epitaxial layers on different off-cut Ge substrates were grown by LP-MOVPE growth and characterized by several characterization techniques. The HRTEM shows the epitaxial growth of GaAs on Ge substrate with well-resolved GaAs lattice lines extending all the way down to the Ge surface. The ECV profile of Si-doped GaAs on 6^o off-oriented Ge substrate shows abrupt film/substrate interface. The excitonic luminescence efficiency from the Si-doped GaAs epitaxial film on 6^o and 9^o off-cut Ge substrates is greater than that from 2^o off-cut Ge substrate. However, the PL spectrum from the GaAs solar cell structure grown on 6^o Ge shows high luminescence intensity than on 9^o off-cut Ge substrate and indicates that the potential use of this off-cut Ge substrate for GaAs space solar cell industry.

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