

## Research Article

# High Quality GaAs Epilayers Grown on Si Substrate Using 100 nm Ge Buffer Layer

Wei-Cheng Kuo,<sup>1</sup> Hung-Chi Hsieh,<sup>1</sup> Wu Chih-Hung,<sup>2</sup> Huang Wen-Hsiang,<sup>2</sup> Chien-Chieh Lee,<sup>3</sup> and Jenq-Yang Chang<sup>4</sup>

<sup>1</sup>*Institute of Materials Science and Engineering, National Central University, Taoyuan, Taiwan*

<sup>2</sup>*Institute of Nuclear Energy Research, Taoyuan, Taiwan*

<sup>3</sup>*Optical Science Center, National Central University, Taoyuan, Taiwan*

<sup>4</sup>*Department of Optics and Photonics, National Central University, Taoyuan, Taiwan*

Correspondence should be addressed to Jenq-Yang Chang; [jychang@dop.ncu.edu.tw](mailto:jychang@dop.ncu.edu.tw)

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We present high quality GaAs epilayers that grow on virtual substrate with 100 nm Ge buffer layers. The thin Ge buffer layers were modulated by hydrogen flow rate from 60 to 90 sccm to improve crystal quality by electron cyclotron resonance chemical vapor deposition (ECR-CVD) at low growth temperature (180°C). The GaAs and Ge epilayers quality was verified by X-ray diffraction (XRD) and spectroscopy ellipsometry (SE). The full width at half maximum (FWHM) of the Ge and GaAs epilayers in XRD is 406 arcsec and 220 arcsec, respectively. In addition, the GaAs/Ge/Si interface is observed by transmission electron microscopy (TEM) to demonstrate the epitaxial growth. The defects at GaAs/Ge interface are localized within a few nanometers. It is clearly showed that the dislocation is well suppressed. The quality of the Ge buffer layer is the key of III-V/Si tandem cell. Therefore, the high quality GaAs epilayers that grow on virtual substrate with 100 nm Ge buffer layers is suitable to develop the low cost and high efficiency III-V/Si tandem solar cells.

## 1. Introduction

Photovoltaics is widely recognized as one of the most desirable options yet suggested for future sustainable energy supply, with on-going cost reduction key to fulfilling this potential. Crystalline silicon solar cell has continued dominating the solar energy market [1]. Yet, III-V solar cell has the highest conversion efficiency in the world [2]. However, this device has high cost, making it difficult to command the solar cell market. Therefore, combining of III-V cells with Si cells does not offer only high performance but also cost reduction. This III-V/Si tandem cells efficiency can be over 40% [2].

Two different process technologies were investigated for the fabrication of III-V/Si tandem cells: direct epitaxial growth and wafer bonding. For example, Derendorf et al. [3] investigate GaInP/GaAs//Si solar cells with three active p-n junctions by surface activated direct wafer bonding between GaAs and Si. The highest efficiency is reached at

71 suns with an efficiency of 23.6%. Even so, direct epitaxial growth process has two advances compared with wafer bonding process, which can have large area production and easy integration with integrated circuit. Nevertheless, large lattice-mismatch and different thermal expansion coefficient between GaAs layer and Si substrate results in high threading dislocations, which influences open-circuit voltage ( $V_{oc}$ ) and carrier lifetime of the cells [4]. Thus, it requires a buffer region to solve the lattice-mismatch problem between GaAs and Si. Ge provides nearly lattice match with GaAs. GaAs growth on Ge/Si virtual substrates was investigated for potential applications of III-V solar cell technology [1, 5–9]. For example, Lueck et al. [6] developed GaInP/GaAs solar cells growth on Ge/Si virtual substrates with efficiencies of 16.8% under AM1.5-G illumination. Diaz et al. [1] presented a GaAsP/SiGe tandem solar cells growths on Si substrates. This tandem solar cells efficiency could reach 18.9% under AM1.5-G illumination.

The quality of the Ge buffer layer is the key of III-V/Si tandem cell. But the Ge layer thickness is also an important issue for the III-V/Si tandem cells. For example, Ichikawa et al. [8] proposed a four-junction III-V/Si tandem solar cell which uses thin Ge buffer layers. In this structure, Ge absorption is dependent on Ge layer thickness and Ge absorption is significantly affecting the bottom Si cell efficiency. However, it is difficult to obtain a Ge epilayer with high crystal quality and thin thickness. Therefore, we used the electron cyclotron resonance chemical vapor deposition (ECR-CVD) to grow the thin Ge epilayer (100 nm) on Si substrates and modulate the hydrogen flow ratio to improve the crystal quality at a low growth temperature of 180°C. Then, GaAs epilayers grow on Ge/Si by metal organic chemical vapor deposition (MOCVD).

## 2. Experimental

Ge epilayers on n-type <100> offcut 6° towards the [110] CZ silicon wafers with resistivity of 1–10 Ω-cm at a low growth temperature of 180°C are obtained using ECR-CVD. Before deposition, the native oxide is removed in a 5% hydrofluoric acid solution. We modulated hydrogen flow rate from 60 to 90 sccm in an attempt to improve crystal quality to obtain epitaxial Ge on Si and the other deposition parameters are as follows: the source gas supplied via an inlet valve upon the ECR region includes Ar and 10% GeH<sub>4</sub> diluted with He; the working pressure is 25 mtorr; the microwave power is 0.14 W/cm<sup>2</sup>. After the deposition, Ge is annealed in a nitrogen atmosphere at 700°C for 5 min to improve the crystallinity. The GaAs layers are grown on Ge/Si by MOCVD. Before GaAs films growth, the Ge/Si sample is baked at 700°C around AsH<sub>3</sub> environment to produce the precursor. The sources gas uses trimethylgallium (TMGa) and AsH<sub>3</sub>; the working pressure is 50 mbar. A 20 nm GaAs seed layer is grown at 450°C on Ge/Si; 2 μm GaAs epilayers are grown at 620°C. The quality of GaAs and Ge films is checked by high resolution X-ray diffraction (XRD) measurement using the incident Cu Kα line as the X-ray source (wavelength is 0.154 nm) at 40 kV and 40 mA to obtain the intensity and the FWHM of the Ge (004) peaks. The deposition and crystallization rate of Ge films are identified by spectroscopy ellipsometry (SE). Transmission electron microscopy (TEM) was used to observe the GaAs/Ge/Si interface to demonstrate the epitaxial growth of Ge on Si.

## 3. Result

Figure 1 shows the XRD rocking curve of the Ge epilayers on Si grown at various H<sub>2</sub> flow rate and we fitted the FWHM of the Ge (004) peaks. We found that, with the increase of H<sub>2</sub> flow rate from 60 to 80 sccm, the FWHM decreases from 993 arcsec to 571 arcsec. Furthermore, the H<sub>2</sub> flow rate increases from 80 to 90 sccm, and the FWHM increases from 571 arcsec to 730 arcsec. The intensity trend is similar to FWHM of the Ge (004) peaks. It is known that the Ge (004) crystal, which is the crystal phase of the epilayer grown on Si, has a better quality at H<sub>2</sub> flow rate which equals 80 sccm. After

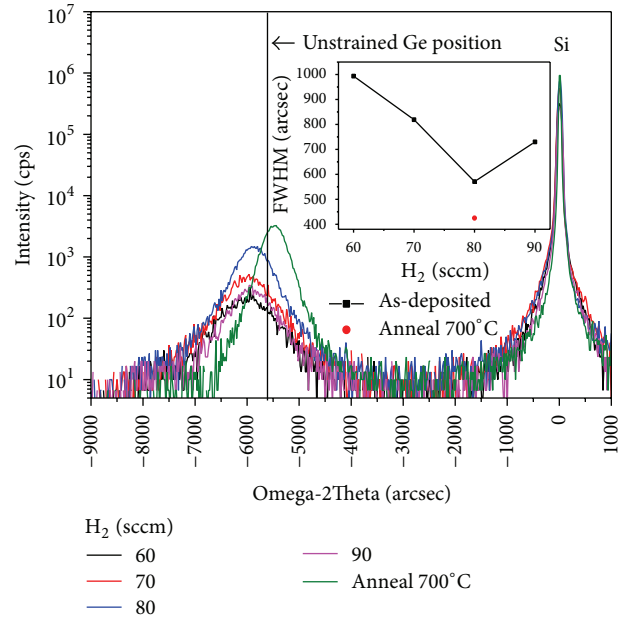


FIGURE 1: High resolution XRD rocking curve of the Ge (004) peak with various H<sub>2</sub> flow rate.

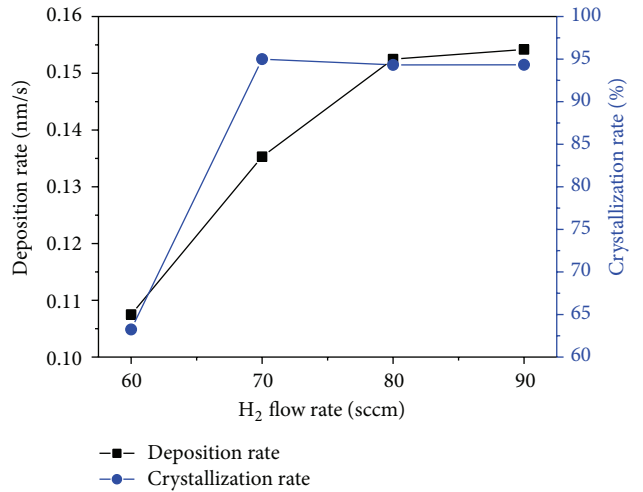


FIGURE 2: The deposition and crystallization rate as a function of H<sub>2</sub> flow rate.

annealing at 700°C, the FWHM of Ge decreases from 571 to 406 arcsec. Figure 2 shows the deposition and crystallization rate of Ge epilayers, measured by SE, as a function of H<sub>2</sub> flow rate. The thickness and crystallization rate of Ge films are fitted by Tauc-Lorentz model and Bruggeman effective medium approximation [10–13]. The Tauc-Lorentz model is given by

$$\varepsilon_2(E) = \begin{cases} \frac{AE_0C(E - E_g)^2}{E[(E^2 - E_2^2) + C^2E^2]}, & \text{if } E > E_g, \\ 0 & \text{if } E \leq E_g, \end{cases} \quad (1)$$

where  $E_g$  is band gap energy,  $E_0$  is energy of maximum absorption (peak transition energy),  $A$  is the amplitude factor

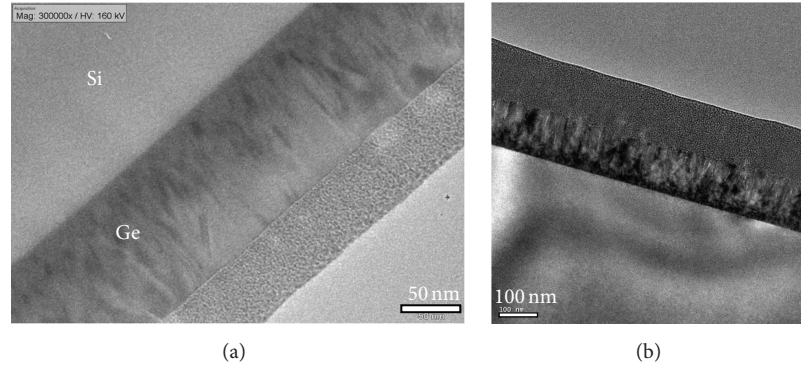


FIGURE 3: High resolution cross-sectional TEM image of the Ge films as deposited at  $H_2$  flow rate of (a) 80 sccm and (b) 60 sccm.

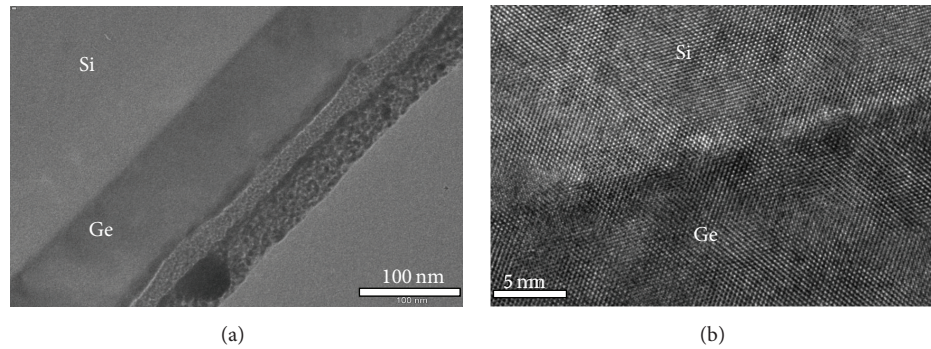


FIGURE 4: (a) High resolution cross-sectional TEM image of the Ge films annealing at  $700^\circ\text{C}$ ; (b) Ge/Si interface.

proportional to the density of the material, and  $C$  is the broadening parameter that is inversely related to the short range order of the material. The deposition rate increases from 0.108 to 0.154 nm/sec as the  $H_2$  flow rate increases from 60 to 90 sccm. Besides, crystallization rate of Ge films is the highest at  $H_2$  flow rate 80 sccm, which is consistent with the Ge quality measurement result of XRD.

Hydrogen adsorption and desorption reactions at Ge film surface are investigated [14]. In addition, the mechanism of passivation of germanium vacancies by atomic and molecular hydrogen has been reported [15]. Appropriate hydrogen can increase the crystallization of the Ge films [16–18]. Therefore, hydrogen passivates dangling bonds and helps Ge-Ge bonds to be stronger when  $H_2$  flow rate is from 60 to 80 sccm. Moreover, an excess of hydrogen in the source gas can etch the film-growing surface and break Ge-H bond [14]. It forms dangling bonds, increasing the damage of the Ge surface. Thus, the Ge films quality tends to decrease when  $H_2$  flow rate is from 80 to 90 sccm.

As the Ge epilayer is observed by SE and XRD, it demonstrates that when the  $H_2$  flow rate is modulated, the crystal quality can be improved. We use TEM to identify the Ge/Si interface epitaxial quality. Figure 3 shows high resolution cross-sectional TEM image of the Ge films as deposited at  $H_2$  flow rate of (a) 80 sccm and (b) 60 sccm. At the Ge/Si interface, Ge epilayers have some dislocation before annealing, the strain originating from the 4.2% lattice

mismatch between Si and Ge leads to islanding accompanied by the formation of misfit dislocations. After that, the Ge films at  $H_2$  flow rate of 80 sccm is annealed at  $700^\circ\text{C}$ . Figures 4(a) and 4(b) show high resolution cross-sectional TEM image of the Ge films annealing at  $700^\circ\text{C}$  and Ge/Si interface. The dislocation of Ge films is decreased, and it is clear that the Ge lattice on the c-Si substrate is epitaxial.

GaAs films quality is dependent on Ge buffer layer quality. After growth of thin Ge buffer layer, we deposit  $2\ \mu\text{m}$  GaAs epilayers on Ge/Si. The GaAs quality is studied by XRD and TEM. The XRD rocking curve of the Ge buffer layer on Si and GaAs epilayer on Ge/Si is shown in Figure 5. In XRD rocking curve, the FWHM of GaAs epilayer is 220 arcsec which is lower than Ge films. To further observe the interface details of the film, we used TEM to distinguish the epitaxial quality of the GaAs/Ge/Si structure of the film as shown in Figure 6. As can be seen, the defects at GaAs/Ge interface are localized within a few nanometers. It clearly shows that the dislocation is well suppressed.

The quality and thin thickness of Ge films are principal for high efficiency III–V/Si tandem cells. But GaAs films grow on Si substrate for numerous investigation uses of thick Ge buffer layer. The XRD FWHM range of GaAs films on Ge/Si is 180–276 arcsec [19–21]. Thick Ge buffer layer can obtain high quality GaAs cells, but it reduces the optical loss of bottom Si cells seriously. In this study, we investigate high quality GaAs epilayers grown on Si substrate using 100 nm Ge buffer layer.



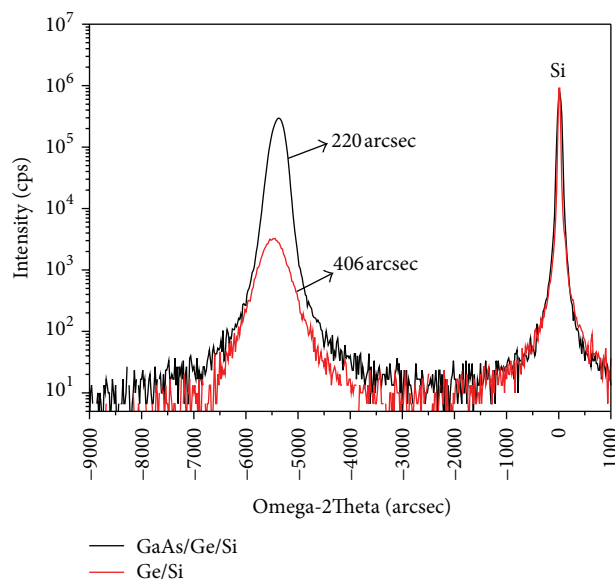


FIGURE 5: High resolution XRD rocking curve of the Ge and GaAs peak.

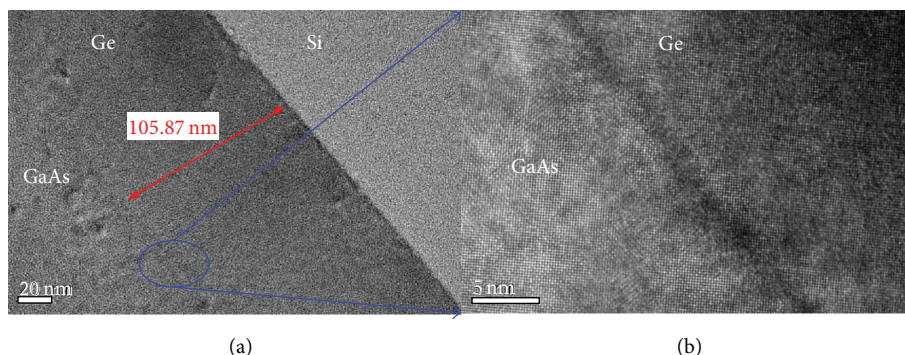


FIGURE 6: High resolution cross-sectional TEM image of the GaAs/Ge/Si (a) interface and (b) lattice.

The XRD FWHM of GaAs is 220 arcsec. This technology be applied to low cost and high efficiency III-V Si tandem solar cell.

#### 4. Conclusion

For the high efficiency III-V/Si tandem cells, Ge quality and thickness are also important. However, it is difficult to obtain a Ge epilayer with high crystal quality and thin thickness. In this study, we used the ECR-CVD to grow the thin Ge epilayer (100 nm) on Si substrates and modulate the hydrogen flow ratio to improve the crystal quality at a low growth temperature of 180°C. The result indicates that the appropriate hydrogen rate can improve the Ge quality. The XRD FWHM of the Ge epilayers is 571 arcsec at  $H_2 = 80$  sccm. Crystallization rate of Ge films is the highest at  $H_2$  flow rate 80 sccm, which is consistent with the Ge quality measurement result of XRD. After annealing at 700°C, the FWHM of Ge was decreased from 571 to 406 arcsec. After growth of thin Ge buffer layer, 2  $\mu$ m GaAs epilayers grow on Ge/Si by

MOCVD. The FWHM of GaAs epilayer is 220 arcsec. An ordered GaAs/Ge/Si interface with epitaxial growth by TEM image can be identified. The quality of the Ge buffer layer is the key of III-V/Si tandem cell. Therefore, the high quality GaAs epilayers grow on virtual substrate with 100 nm Ge buffer layers for low cost and high efficiency III-V/Si tandem solar cells were developed and demonstrated.

#### Competing Interests

The authors declare that they have no competing interests.

#### Acknowledgments

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