High-quality Ge epilayers grown on a Si substrate in one step process via hot wire chemical vapor deposition

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Abstract. High-quality Ge epilayers on Si with a low threading-dislocation density (TDD) were grown by a one step hot wire chemical vapor deposition process at 350°C without cyclic thermal annealing. The Ge layers with threading dislocation density (TDD) of 1·10⁵ cm⁻² for a 1.4 μm thick Ge layer were obtained on Si wafers of a diameter Ø = 5 cm. Root mean square of roughness (RMS) of ~ 0.37 nm is achieved. The Ge layers produced are of high optical quality.

1. Introduction
Epitaxial growth of fully relaxed Ge epilayers on Si substrates is of current interest for a number of new technologies, such as high performance Ge-on-Si photodetectors for infra-red sensing, solar cells, optoelectronics or Ge lasers [1]. These technologies all benefit from being compatible with the Si(001) substrate. Furthermore, successful growth on Si provides a virtual substrate for the integration and fabrication of GaAs-based optical devices on Si. The epitaxial growth is usually performed by ultra-high vacuum chemical vapor deposition (UHV-CVD) or molecular-beam epitaxy (MBE). However, these methods operate under an ultra-high vacuum atmosphere. On the contrary, chemical vapor deposition (CVD) offers such advantage as high throughput.

Growth of epitaxial Ge on Si at low substrate temperature by hot wire (HW) CVD has been reported in [2]. However, at a lower substrate temperature Tₛ = 350°C Mukherjee could grow only the 300 nm thick epitaxial Ge film. The main advantage is that this technique is relatively simpler than MBE and UHV CVD.

Here we report the growth of relatively thick (with a thickness of about 0.2 – 5 μm and above) epitaxial Ge films on (001) oriented c-Si wafers by HW CVD.

2. Experimental details
The samples were prepared on 5 cm diameter n-type (001) Si wafers with a resistivity of 5 – 10 Ω·cm by HW CVD with a base pressure of 5·10⁻⁸ torr [3]. After standard RCA etching and thermal cleaning of Si substrate at 900°C for 20 min, a 200 nm thick Si buffer layer was grown at 800°C. Then a Ge-film was grown at 350°C. The deposition of Ge was carried out by letting purified germane (GeH₄) inside the growth chamber through a leak valve. The partial pressure of GeH₄ was 4·10⁻⁴ Torr. Germane was cracked pyrolitically on a tantalum wire heated directly by passing the direct electric current through the wire up to 1200 - 1300°C.
The Ge films were grown at the same growth conditions as the Ge/n+-Si(001) structures for the fabrication of the photodiodes. The surface morphology of the Ge/Si(001) layers was examined by Atomic Force Microscopy (AFM) in ambient air using a NT-MDT Solver ProTM instrument. The crystal structure of the Ge/Si(001) films was examined by Double crystal X-Ray Diffraction (DXRD) and by Transmission Electron Microscopy (TEM). The X-ray diffraction experiments have been carried out using a Bruker D8 Discoverer TM X-ray diffractometer with CuK radiation. TEM investigations have been carried out using a JEOLJEM 2100F transmission electron microscope.

3. Results and discussion
Figure 1 shows typical optical image of TDD in a Ge epilayer on a Si substrate. The typical TDD in ~1.4 μm thick layers is in a range of 1·10⁵ cm⁻². Notice that TDD of Ge epilayers of the same thickness obtained by the RP CVD method was 10⁷ - 10⁸ cm⁻² even after thermal annealing [4].

![Figure 1. Optical image of a Ge epilayer on a Si substrate after etching by I₂ solution](image)

XRD ω-2θ scans around Si(400) and Ge (400) diffraction of a 1μm thick Ge layer are shown in figure 2. The crystallinity of the Ge layer was approved by the presence of an intensive Ge(004) peak. The sample shows a nearly symmetric Ge (400) peak including no detectable diffusion between Ge and Si. The full width at half maximum (FWHM) of the Ge peak is 0.052°.
Figure 2. HR XRD 2θ scan profile of a Ge film on a Si substrate, grown at 350°C substrate temperature.

Cross-sectional TEM of the heteroepitaxial Ge films of ~ 1 μm shows a high density of threading dislocations confined to a region ~ 0.2 μm wide adjacent to the Ge/Si interface (figure 3(a)).

High resolution images were also observed in the interface region between the Si substrate and the Ge film (figure 3(b)). The continuous crystalline structures are clearly seen at the Ge/Si interface and thus the epitaxial growth following the substrate is confirmed.

Figure 3. The cross-sectional TEM image of a Ge film on a single crystal Si(100) substrate: (a) TEM image observed in the whole thickness (b) the interface region between the Si(100) substrate and the Ge film.
Figure 4 shows the atomic force microscope (AFM) image of a Ge epilayer on a Si substrate. The surface is found to consist of step and terrace structures, indicating the two-dimensional layer-to-layer growth. A small RMS surface roughness of 0.37 nm is obtained.

![AFM image of Ge epilayer on Si substrate](image)

**Figure 4.** A morphology of a Ge epilayer on a \( \sim 0.25 \mu \text{m} \) thick Si substrate.

A spectral dependence of the external photoelectric quantum efficiency \( \eta \) of a photodiode based on a Ge/Si heterostructure is presented in figure 5. The photodiode demonstrated a good photoresponse in the 1.1 - 1.5 \( \mu \text{m} \) wavelength band.

![Spectral dependence of external photoelectric quantum efficiency](image)

**Figure 5.** The spectra of the external photoelectric quantum efficiency (300 K) of a photodiode based on a Ge/Si(001) heterostructure measured at different values of reverse bias \( U_b \).

Although this value is \( \approx 4 \) times lower than the highest ones reported in the literature, there is still a wide room for further improvement of the quantum efficiency. High crystal quality of Ge layers on Si(100) substrates can be explained.
When using the low temperature HW CVD method, the hydrogen injection into a Ge layer with formation of clusters occurs. Low diffusion barrier promotes the diffusion and surface mobility of adatoms, which facilitates Ge relaxation and reduces the density of defects caused by the lattice mismatch.

4. Conclusion
In summary, a virtual Ge template composed of a Ge epilayer on a Si substrate can be obtained in one step process via the HW CVD method without UHV condition. The high-quality 0.2 – 5 μm thick Ge epilayers on Si with a surface RMS roughness of about 0.37 nm and TDD of $1 \cdot 10^5$ cm$^{-2}$ were obtained. HW UHV CVD has been demonstrated to be a promising method for fabrication of the Ge/Si(001) photodetectors used in the Si-based electronic-photonic integrated circuits. Those results suggest that Ge will play a significant role as an enabler for integrated active photonic devices on Si.

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