*Proceedings of the International Conference*
*Nanomaterials: Applications and Properties*
Vol. **2** No 1, 01PCSI20(4pp) (2013)

# Study of Structure and Intrinsic Stresses of Ge Thin Films on GaAs

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(Received 13 June 2013; published online 01 September 2013)

The effect of film growth rate on the structure and intrinsic stresses of thin (~100 nm) Ge films grown on GaAs(100) substrates was investigate by High Resolution X-Ray Diffraction (HRXRD). The Ge films were deposited onto GaAs using thermal evaporation of Ge in the vacuum. It was shown that pseudomorphic films with good structural quality can be obtained by this growth technique. We found out that the films have biaxial deformations due to coherent interface and Poisson ratio. The films are elastically compressed in the interface and stretched in the perpendicular [001] direction. The intrinsic deformations of thin Ge films strongly depended on the deposition rate. Their correlations with surface roughness, electrical and optical parameters are discussed.

**Keywords:** Ge/GaAs, High resolution X-ray diffraction, Intrinsic stresses

PACS numbers: 61.05.cp, 68.55.– a

## 1. INTRODUCTION

The Ge/GaAs heterostructure is promising for a number of practical applications such as high-performance solar cells [1-4], metal oxide semiconductor field-effect transistors [5, 6], microwave diodes [7], and sensors, e.g. thermometers [8, 9], and -ray and optical radiation detectors [8, 10-13]. In addition the Ge/GaAs is an excellent model system for IV/III-V heterostructures in general. This heterostructure is characterized by close values of the components lattice constants as well as practical coincidence of their thermal expansion coefficients [1]. These properties are favorable for epitaxial growth and fabrication of films and heterojunctions with almost perfect structure.

The defect formation in the Ge/GaAs heterostructures depends on which material serves as the substrate (Ge or GaAs). In this work, we consider Ge film epitaxy on the GaAs(100) substrate.

The Ge lattice constant exceeds that of GaAs. Therefore, the Ge films grown on GaAs substrates are compressed. It was experimentally shown [14] that elastically compressed Ge films on GaAs may exist up to film thickness of 5 μm. In that case, there are no mismatch dislocations which could impair the electrical properties of the heterojunction. Thus, it is possible to form a high-quality interface (without misfit dislocations) in the Ge/GaAs heterostructure.

The distinguishing feature of Ge films on GaAs is the strong dependence of their structural, electrical and optical properties, on the method of preparation. This is related to possible interdiffusion of the joining materials [15-23]. For Ge films, diffused Ga and As atoms act as shallow acceptors and donors, respectively. Therefore, because of autodoping, the Ge films on GaAs may be *p*- or *n*-type with different degrees of compensation including fully compensated [8, 24-27]. Moreover the degree of structural perfection of the Ge films, as well as the concentration of structural defects in them, is determined by the film preparation condition. The Ge films can be amorphous, poly- or single crystalline, with different degrees of structural perfection.

The pioneer work on fabrication and investigation of the Ge/GaAs heterostructure can be traced to the paper by Anderson [28]. A rather large number of studies has been done to understand the effect of factors such as: preparation methods, substrate temperature, film thickness and GaAs surface preparation on the growth mechanism [29-37], surface and heteroboundary morphology [15, 23, 36-43], intrinsic stresses [12, 33, 39-42], electrical [15, 23, 28, 40, 46-48] and optical [23, 28, 46, 49] properties of Ge films on GaAs. However, the effect of the deposition rate on the properties of Ge films on GaAs remains not fully explored, with few studies considering only high deposition rates [50, 51].

In our previous [8, 24] and recent work [26, 27, 52] we show that deposition rate drastically affects the electrical and optical properties as well as surface morphology of thin (~100 nm) Ge films on GaAs. In particular we show that efficient control of the film properties can be achieved by varying their deposition rate.

The subject of this paper is further in-depth study the effect of film growth rate with focus on structure and intrinsic stresses of thin Ge films by using High Resolution X-Ray Diffraction (HRXRD). Measured rocking curves show that pseudomorphic samples with good structural quality can be obtained by this growth technique. It was also shown that the films are elastically compressed and intrinsic stresses strongly depended on the deposition rate.

## 2. PREPARATION CONDITIONS AND MEASUREMENT PROCEDURE

The Ge films were deposited using thermal evaporation of Ge in the vacuum ($2\times10^{-4}$ Pa) onto semi-insulating ($10^7$ Ω·cm) GaAs(100) substrates. The temperature of GaAs substrate during the film deposition was maintained at 500 °C. The film deposition rate was maintained constant over the course of each deposition; and varied (0.02–0.35) nm/s for different specimens. The evaporation source was a glass-graphite crucible

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heated with electric current flowing through it. The deposition rate was set by the crucible current that determined the Ge evaporation temperature. The film thicknesses were 100±20 nm. Before Ge film deposition, the GaAs substrates were treated with the $H_2SO_4$:$H_2O_2$:$H_2O$ = 4:1:1 etchant for 3 min. and thermal annealed in vacuum at 500 °C for 15 min.

The structural quality of Ge/GaAs heterostructure was studied by HRXRD using a Philips MRD diffractometer with a Cu anode X-ray beam. The X-ray source was operated at 40 kV and 40 mA. A four-crystal Bartels monochromator was employed using four Ge 022 reflections to provide a monochromatic beam with a divergence of 12 arcsec.

The intrinsic stresses ($\sigma$) due to lattice mismatch between Ge and GaAs also were determined from the radius of curvature of specimen surfaces using a profilograph and by application of the Stoney's formula [53, 54], $\sigma = Et^2/[6(1-\nu)Rd]$ where $E$, $t$ and $\nu$ are Young's modulus, thickness and Poisson ratio of the substrate, respectively, $d$ is the film thickness and $R$ is the heterosystem bending radius.

## 3. EXPERIMENTAL RESULTS AND DISCUSSION

### 3.1 Structure and Intrinsic Stresses

Fig. 1 shows the experimental and simulated rocking curves (004 reflection) for Ge/GaAs films obtained at different growth rates. One can clearly observe the Bragg peaks for Ge and GaAs substrate. The Ge films are pseudomorphic. The in-plane Ge lattice constant is very close to that of GaAs, with corresponding lattice constant increasing in the perpendicular direction. The left-side shift of Ge film maximum in comparison with a bulk Ge single crystal is observed (Fig. 1). The vertical dotted lines in Fig. 1 indicate the diffraction angle position for bulk Ge.

At low deposition rate, the absence of interference fringes and higher intensity of tails are caused by some structural inhomogeneities of the film and interface roughness that were not taken into account at simulations.

At high growth rate, the interference fringes in the Ge film are observed (Fig. 1(b)), thus indicating phase coherency of the diffracted waves and high crystalline quality of this heterostructure.

The investigations of radius of curvature of the Ge/GaAs heterostructure showed that Ge films are compressed. The intrinsic stresses in the Ge films about 100 nm thick also calculated using the Stoney's formula are at the level of several tenth parts of GPa. They depend on the film growth rate, decreasing from $6.7\times10^8$ Pa to $2\times10^8$ Pa (i.e. by more than three times) as the deposition rate decreased from 0.35 nm/s to 0.02 nm/s (Fig. 2).

### 3.2 Surface Roughness, Electrical and Optical Parameters

In our recent work [27, 52] we show that deposition rate also strongly affects the surface morphology, electrical and optical properties of the Ge films.

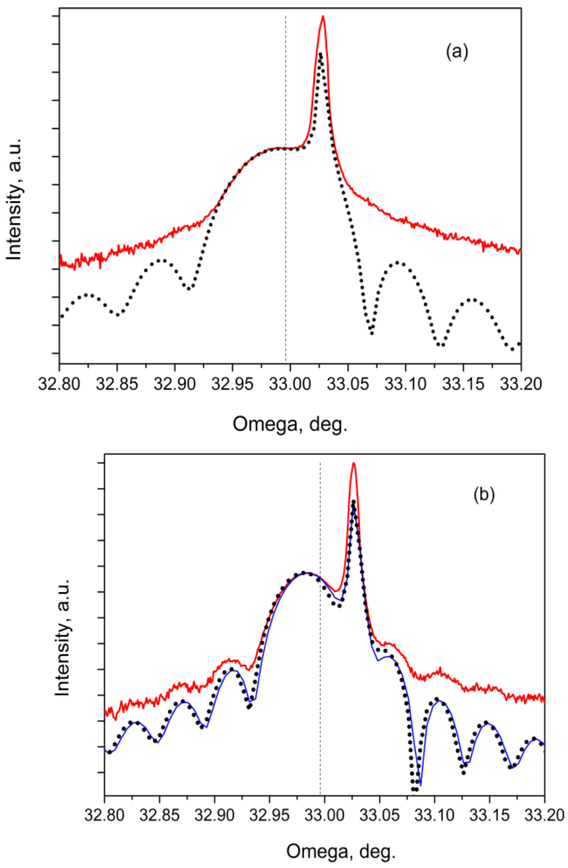

**Fig. 1** – Rocking curves (004) for Ge films on GaAs. The film thickness was 100±20 nm. Ge growth deposition rates used are 0.02 nm/s (a) and 0.35 nm/s (b). Vertical dotted line denotes position of diffraction maximum from the bulk Ge. Simulated dotted curves correspond to ideally pseudomorphic film. The blue curve in (b) is simulation fitted to experimental data

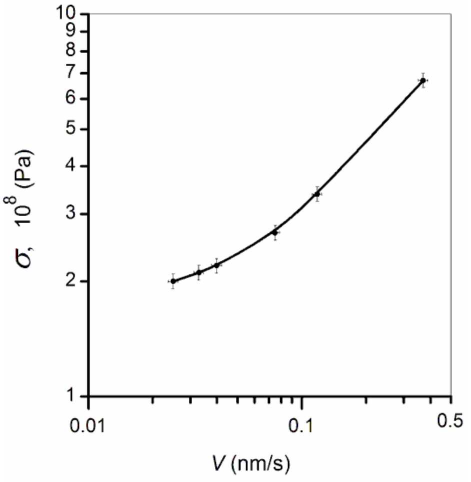

**Fig. 2** – Dependence of intrinsic stresses ($\sigma$) in Ge films on GaAs on the film growth rate ($V$). The film thickness was constant (about 130 nm)

The films prepared at high deposition rate have smooth surfaces with root-mean-square (RMS) roughness of about 0.5 nm. In contrast, at low growth rate film roughness is large and can reach up to 14.6 nm in the film of 100 nm thick.

Optical absorption measurements of the Ge films show that at energies $E < E_g$, the optical absorption coefficient $D$ depends on the photon energy $E$ as $D \approx \exp[-(E_g - E)/\Delta]$, where $\Delta = dE/d\ln D$ is the characteristic energy that determines the spreading of the fundamental absorption edge. For the Ge films in this study Δ does not depend on temperature. This exponential dependence $D(E)$ is related to the tails in the density-of-states in the Ge band gap. The existence of these tails permits optical transitions at photon energies below $E_g$. Table 1 presents the Δ values for films obtained at different deposition rates. As the deposition rate decreased, the tails in the density of states, and thereby the Δ value, increased. The degree of spreading of the fundamental absorption edge Δ can be varied from 60 meV up to 140 meV.

**Table 1** – Dependencies of intrinsic stresses (σ), characteristic energy Δ, resistivity (ρ), activation energy of conductivity ($\varepsilon_1$), conductivity type and root-mean-square (RMS) roughness for the Ge films of 100±20 nm thicknesses grown at different deposition rates $V$.

| **V** (nm/s) | 0.02 | 0.35 |
|---|---|---|
| **σ** (Pa) | $2\times10^8$ | $6.7\times10^8$ |
| **RMS** (nm) | 14.6 | 0.49 |
| **ρ** (Ω/cm) | 120 | 0.02 |
| $\varepsilon_1$ (eV) | 0.35 | 0 |
| Conductivity type | p | n |
| **Δ** (meV) | 140 | 70 |

The transport phenomena in Ge films obtained at low and high deposition rate also differ drastically. The Ge films obtained at high deposition rate are *n*-type, low-resistant (0.1-0.01 Ω·cm), heavily doped and slightly compensated (Table 1). Temperature dependence of conductivity in these films is weak or practically absent. The films obtained at low deposition rate are *p*-type, high-resistant (~100 Ω·cm), heavily doped, and strongly compensated; in the limiting case fully compensated. Their conductivity is thermally activated. The activation energy of conductivity can reach up to half of the Ge band gap (Table 1).

## 4. CONCLUSION

We present a HRXRD study of Ge/GaAs thin films. The measured rocking curves show that an ideally pseudomorphic growth of Ge films with good single crystal structure can be obtained by this growth technique. The film-substrate interface is coherent and dislocation free. It was also shown that the films are elastically compressed and intrinsic stresses strongly depend on the deposition rate. This effect is essential and should be taken into account when developing and producing devices based on the Ge/GaAs heterostructure.

## AKNOWLEDGEMENTS

This work was partially funded under the Ukrainian State Program “Nanotechnologies and nanomaterials”, Projects No. 2.2.6.15 and 3.6.1.10.

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