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Structural study of Ge/GaAs thin films

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Abstract. Ge/GaAs heterostructure research is largely motivated by the application of this material in solar cells, metal—oxide—semiconductor field-effect transistors, mm-wave mixer diodes, temperature sensors and photodetectors. Therefore, understanding of how the properties of Ge/GaAs heterostructure depend on its preparation (growth) is of importance for various high-efficiency devices. In this work, by using thermal Ge evaporation on GaAs(100), we studied structural properties of these films as a function of the deposition rate. Film grains size and morphology show strong dependence of the deposition rate. Low deposition rates results in films with large crystal grains and rough surface. At high deposition rates films become flatter and their crystal grains size decreases, while at very high deposition rates films become amorphous. Cross-sectional TEM of the films show that the Ge films are granular single crystal epitaxially grown on GaAs. The Ge/GaAs interface is atomically abrupt and free from misfit dislocations. Stacking faults along the [111] directions that originate at the interface were also observed. Finally by using the Kelvin probe microscopy we show that work function changes are related to the grain structure of the film.

1. Introduction

The study of Ge/GaAs heterostructure is largely motivated by application of this material in various solar cells, metal–oxide–semiconductor field-effect transistors, mm-wave mixer diodes, temperature sensors and photodetectors. Therefore, information on how the properties of Ge/GaAs heterostructure depend on its preparation conditions is of importance for the application of this system in various high-efficiency devices. The studies of growth mechanisms of thin Ge films on GaAs [1-5] show that Ge films grow on GaAs (100) in the layer-by-layer (Franck-van der Merwe) mode at temperatures below about 400 °C, whereas at higher temperatures growth occurs by the island (Stranski-Krastanov) growth mechanism. Numerous studies have been reported on the influence of the substrate temperature and the GaAs surface composition on the electrical properties of Ge films and heterojunctions [1, 6–9]. However, the effect of the deposition rate on the properties of thin Ge films on GaAs has not been investigated thoroughly; in most of the reports rather high film deposition rates have been chosen as a rule. Recently we have demonstrated that by varying the deposition rate of Ge/GaAs one can control the transport properties effectively [10]. The high deposition rates produce films that are n-type doped with low resistivity ($10^{-2} \ \Omega$ -cm) and high carrier concentration ($4 \times 10^{18} \ cm^3$). The temperature dependence of conductivity in these films is very weak and of non-activation

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type, indicating metallic like transport with degenerate charge carriers. In contrast, low deposition rates produce single crystal films with larger grains that are p-type doped with high resistivity ($10^2 \, \Omega \cdot \text{cm}$) and low carrier concentration ($10^{15} \, \text{cm}^3$) [10]. In this work we present a structural study of thermally deposited Ge/GaAs films by transmission electron microscopy (TEM) and atomic force microscopy (AFM).

2. Experiment

The films were deposited on GaAs(100) substrates using thermal evaporation of Ge in the vacuum. The temperature of GaAs substrate remained constant (490 ± 10 °C) during the Ge film deposition. The deposition rate (from 0.025 to 0.37 nm/s) was controlled by varying the temperature of Ge crucible. Films surface morphology has been investigated by AFM. Bright field (BF) TEM imaging and selected area diffraction (SAD) has been performed by JEOL 2011. The high resolution TEM (HRTEM) and high angle annular dark filed imaging has been done by the double aberration corrected JEOL 2200 FS microscope. Scan-line energy dispersive X-ray analysis was performed by using the Thermo-EDX system. TEM cross-section specimens were prepared by gluing the films' sides with a Gatan G1 epoxy resin. Mechanical thinning followed by polishing was carried out until ~20µm specimen thickness. The final step included Ar ion milling by using Gatan PIPS ion miller in order to achieve electron transparency. Initial ion-milling parameters were set as the following: ion beam energy 3keV with 5^0 angles with respect to the bottom and top of specimen surface; at the final stage of ion milling the energy of the beams was decreased to 2.5 keV and angles to 4^0 .

3. Results and Discussion

Both GaAs and Ge have cubic (zinc-blende) structure with lattice constant of 5.6533 Å and 5.6461 Å , respectively. The same crystal structure and the very small difference in the lattice constants make these two materials almost an ideal epitaxial match, with mismatch of only -0.12 %. Indeed the deposited Ge films are single crystal, as confirmed by the SAD from the Ge film (Figure 1). The epitaxial relation between the film and the substrate is a simple cube on cube relation; $Ge(001)\|GaAs(001)$ and $Ge(100)\|GaAs(100)$. The AFM surface morphology and the BF-TEM clearly show that the growth is in Stransky-Krastanov (3D) mode with the grain size of ~75 nm (Figure 1a and b).

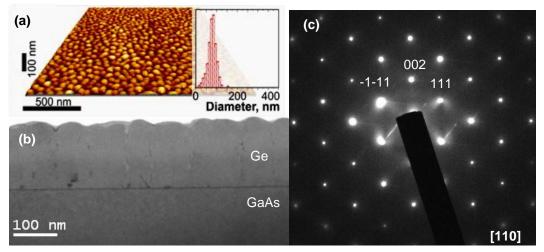


Figure 1. a) AFM showing surface topology of Ge/GaAs films deposited at 0.37 nm/s. b) BF cross-section TEM of Ge/GaAs, and (c) SAD from the Ge film.

The interface between Ge and GaAs appears to be well defined; interface roughness (up to 1 nm) can be seen from the HTREM images (Figure 2a). The high resolution (HR) HAADF imaging supports this observation (Figure 2b); though a small amount of waviness is present at the interface. This

indicates possible atomic mixing at the interface region. The scan line EDX across the interface also suggest that such mixing could happen, though due to the beam spread and the size of interface region this should be examined by additional methods in order to fully verify the presence of atomic mixing at the Ge/GaAs interface. The BF-TEM (Figure 1b) as well as HAADF (Figure 3a) show presence of linearly shaped defects that starts at the interface and extend in the Ge film for several tens of nm. The HAADF (Figure 3c) and the HRTEM (not shown here) clearly show that these defects are twin stacking faults (SF). The SF occurs on the {111} type of planes, and they vary in their width from several to tens of atomic planes. All the SF faults originate at the interface and at small number of SF we observe presence of dislocation(s), either at the Ge/GaAs interface or along the twin mirror plane of the SF.

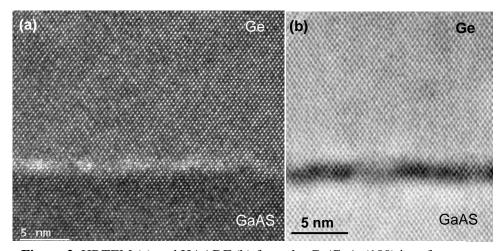
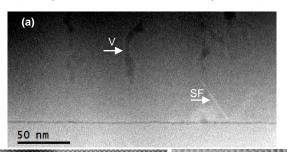


Figure 2. HRTEM (a) and HAADF (b) from the Ge/GaAs(100) interface.

In addition to the SFs, Ge grain boundaries are clearly seen in BF-TEM and HAADF (Figure 1b and Figure 3a, respectively). Regions with white (dark) contrast are observed along these boundaries in BF (HAADF) images. The HR-HAADF (Figure 3c) shows that these dark contrast regions are fully



crystalline; the darker contrast most likely originates from the presence of voids along the grain boundaries, thus these regions appear darker in the Z-contrast imaging. The void formation is believed to be a result of the 3D columnar growth of the Ge film.

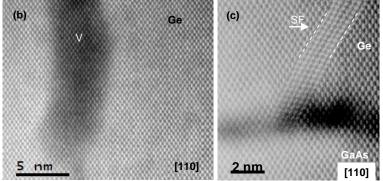


Figure 3. a) HAADF from the the Ge/GaAs film. b) HR- HAADF from the grain boundary regions (b) where voids (V) are present. c) HR-HAADF from twin stacking fault that originates at the Ge/GaAs interface.

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The importance of the Ge grain boundaries and their possible role in the outdiffusion of Ge/As in the film (and ultimately the Ge films conductivity) is illustrated in Figure 4. The surface topography of low rate deposition Ge film (Figure 4a) and the corresponding surface potential mapping by Kelvin probe AFM (Figure 4b) show good correlation. The changes of the surface potential coincide with the Ge grain boundaries indicating that the outdiffusion of Ga(As) can be significant along the grain boundaries.

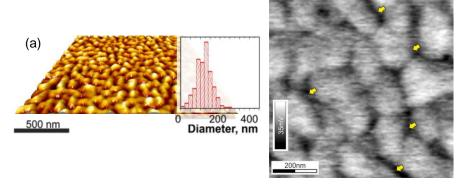


Figure 4. a) Surface topology of low deposition rate (0.04 nm/s) Ge film. b) Surface potential map, the regions with lower work function are marked with arrows.

4. Conclusions

We present a TEM/AFM study of the Ge/GaAs films. The 3D growth of Ge film results in single crystal epitaxial films on GaAs(100). The film-substrate interface is sharp and presences of twin stacking faults have been found in the interface region. No defects have been observed at Ge grain boundaries, the darker HAADF contrast at these boundaries is most likely due to the voids. These boundaries can have significant role in the Ga(As) outdiffusion from the substrate into the Ge film.

Acknowledgments

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