

GaAs/Ge Crystal Growth on Ta₂O₅-Coated Si Substrates

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GaAs/Ge single crystals are grown on insulator-coated Si substrates using the laterally seeded zone melting method in combination with MOCVD. Tantalum pentoxide (Ta₂O₅) is chosen as an insulator instead of the more widely used SiO₂ because of its good molten Ge wettability on the surface. Results confirm that the GaAs/Ge grown on Ta₂O₅ exhibits a crystallinity superior to that obtained on SiO₂. Ge wettability at the Ge/insulator interface is found to be a significant factor in obtaining not only large-area growth but also high crystal quality.

§1 Introduction

Single-crystal GaAs growth on insulator-coated Si substrates is of considerable interest for its application to opto-electronic devices.^{1),2)} In line with this, Ge crystal serves a useful buffer layer between GaAs and insulator because of its good lattice constant and thermal expansion coefficient matching to GaAs crystal. Ge crystal growth on insulators has been studied by several researchers using zone melting crystallization with strip heater systems,³⁻⁵⁾ or scanning laser beam systems.⁶⁾ Thin tungsten (W) film-coated SiO₂ layers have been used as an underlayer for Ge-on-insulator fabrication.^{5),7)} W is used primarily because it promotes molten Ge wettability which is instrumental in preventing the beading up of molten Ge and in obtaining large-area crystal growth up to several hundred micron size.

Significant problems remain, however, with insulation and transparency from the device application viewpoint. Ge-wettable transparent insulator materials are thus essential for underlayer use. Consideration of these conditions led to selecting tantalum pentoxide (Ta₂O₅) to serve as the new insulator films.

This paper demonstrates that Ta₂O₅ is a suitable material for use as an underlying insulator and that single-crystal GaAs/Ge layers grown on Ta₂O₅-coated Si substrates exhibit high-quality characteristics. The crystal quality improvements are discussed on basis of the wettability.

§2 Experimental

Ge wettability on Ta₂O₅, SiO₂, and W was evaluated through contact angle measurement prior to Ge crystal growth. Ge deposited on these films was melted in ambient H₂ and then cooled to room temperature. The contact angles of the frozen Ge on these films were measured directly from SEM photographs.

Ge crystals were grown by laterally seeded zone melting crystallization.⁷⁾ The substrates used in this experiment were (100)Si overcoated with 0.1 μm thick Ta₂O₅ films deposited by RF sputtering in Ar 80% + O₂ 20% ambience. Thermally grown 0.1 μm thick SiO₂ films and electron-beam (EB) evaporated 0.03 μm thick W on SiO₂ were also used for underlayers to provide a means for comparing the Ge crystal qualities obtained. After 50 μm wide stripe seeding openings oriented along the <110> direction were formed, and 300 × 300 μm² insulator areas were defined, 1 μm thick Ge and 0.06 μm thick W layers were deposited by EB evaporation. The W layer was used as a capping layer for promoting large-area crystal growth. The zone melting crystallization of the Ge films were carried out by passing the sample under a carbon strip heater in ambient H₂.

Heteroepitaxial GaAs layers were subsequently grown on the Ge films at about 640 °C using conventional atmospheric pressure MOCVD systems.⁸⁾ Trimethylgallium (TMG) and arsine (AsH₃) were used as source gases. The growth rate was 0.03 μm /min, with the final film thickness being 2 μm.

The sample surfaces were observed with a Nomarski

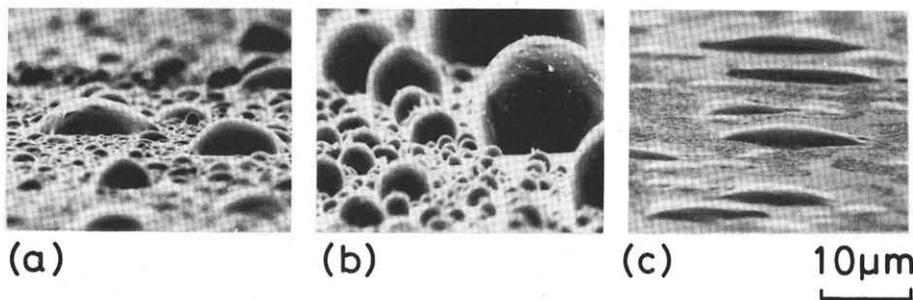


Fig. 1 SEM photographs of Ge melted on Ta₂O₅ (a), SiO₂ (b) and W(c).

optical microscope following chemical etching of the W capping layer. The Ge crystal qualities were studied by double crystal x-ray diffraction and etch pit observation. The GaAs layers were evaluated by cathodoluminescence measured at 40 K.

§3 Results and discussions

Figure 1 compares the wettability states of Ge on Ta₂O₅, SiO₂, and W. The contact angles between the frozen Ge and the films were respectively measured to be about 45° for Ta₂O₅ (a), 110° for SiO₂ (b), and 15° for W (c). This comparison clearly indicates that Ta₂O₅ has a greater Ge wettability advantage than SiO₂, and that its wettability compares to that of W. From the good Ge wettability on Ta₂O₅, maintaining fairly flat surfaces should be possible during laterally seeded Ge crystallization.

Figure 2 depicts typical surface micrographs of the crystallized Ge after removing the W capping layer. A smooth and planar Ge growth was obtained on Ta₂O₅ islands as large as 300 × 300 μm² (Fig.2 (a)), whereas line-shaped voids and relatively rough surfaces were observed in Ge crystallized on SiO₂ islands (Fig.2 (b)).

Double crystal x-ray diffraction rocking curves of (400) planes of Ge crystallized on Ta₂O₅, SiO₂, and W are shown in Fig. 3. The full width at half maximum (FWHM) of Ge/Ta₂O₅ and Ge/W have much smaller values (420 sec and 390 sec in arc) than that of Ge/SiO₂ (730 sec in arc). This implies that the formers have crystallographically better characteristics than the latter.

The cathodoluminescence spectra at 40 K for the GaAs layers grown on Ge/Ta₂O₅ and Ge/SiO₂ islands are compared in Fig. 4. It can be seen that the intensity of the luminescence around 0.84 μm due to the near band edge emission from GaAs on Ge/Ta₂O₅ is 5

times larger than that from GaAs on Ge/SiO₂. This result indicates that the crystal quality of GaAs is considerably improved in crystals grown on Ge/Ta₂O₅. The good GaAs layer crystal quality stems directly from the flat, crystallographically good underlying Ge layers. The broad emission spectra around 1.1 μm are most probably due to defects. Although the luminescence properties of GaAs on Ge/Ta₂O₅ was superior to that on SiO₂, its intensity was still smaller than that of GaAs/GaAs homoepitaxial crystals. This probably results from the existence of antiphase domains which were found by optical microscope observation of the GaAs surfaces.

The experimental results show that the Ge crystal quality strongly depends on the underlayer material properties. Physical factors which affect the crystal quality can be discussed in terms of three components: (1) the residual stress in crystallized Ge, (2) the latent heat liberation accompanied with the crystallization of molten Ge, and (3) the wettability.

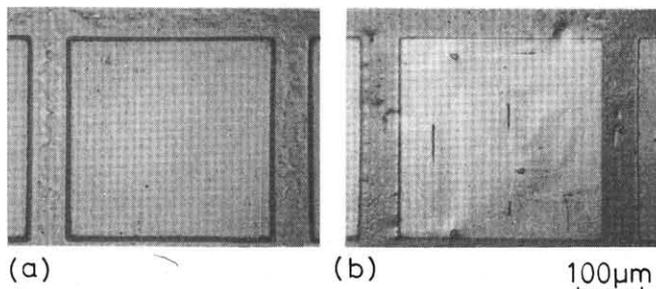


Fig. 2 Nomarski photographs of Ge surfaces crystallized on Ta₂O₅ (a) and SiO₂ (b).

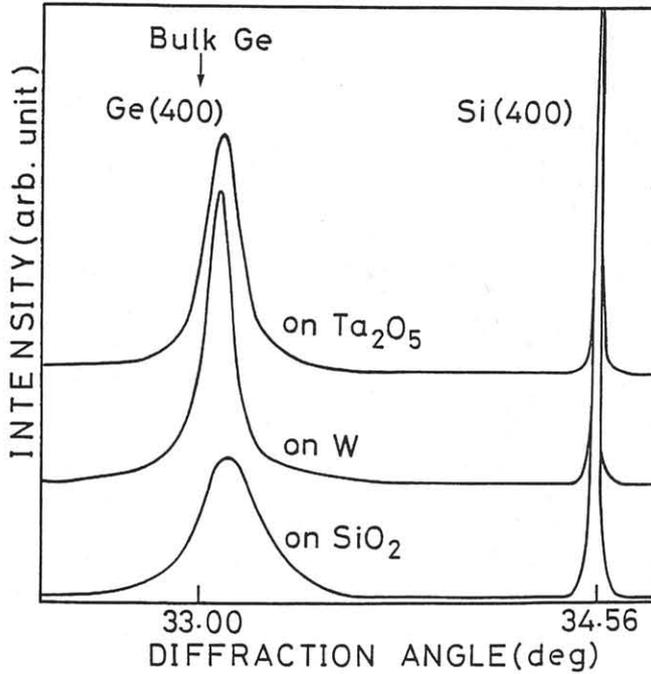


Fig. 3 Double crystal x-ray diffraction profiles reflected from (400) planes of Ge films and Si substrates. X-ray source is $\text{Cu K}\alpha_1$.

The stress can be estimated by the (400)Ge peak shift of the x-ray diffraction curves, shown in Fig. 3, and found to be about $3 - 4 \times 10^9 \text{ dyne/cm}^2$ in tensile for all samples. The stress is considered to be caused by the thermal expansion difference between the Ge and Si substrates.⁵⁾ This indicates that all samples in our experiments are under equal conditions as far as the residual stress in the crystallized Ge is concerned.

The liberation of the latent heat accompanying crystallization is well known to affect crystal quality.^{9),10)} If the latent heat is not released smoothly from the crystal/liquid interface, high-quality crystallization will not be successfully achieved, and defects will be introduced into the growing crystals. In our experimental procedure, three channels existed for the latent heat liberation: (1) liberation to the H_2 atmosphere through the W capping layers, (2) liberation to the Si substrates along the crystallized Ge, and (3) liberation to the Si substrates through the underlayers. The influence of channels (1) and (2) is thought to be similar for all the samples, because the zone melting crystallization was performed each time under the same growth condition.

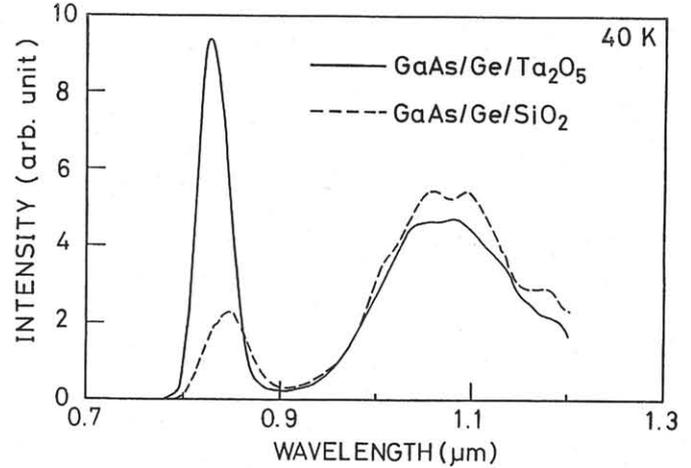


Fig. 4 Cathodoluminescence spectra of GaAs grown on Ge/ Ta_2O_5 (solid line) and on Ge/ SiO_2 (dashed line).

The heat conduction of channel (3) will vary depending on the underlayer material and structure. To distinguish the wettability effect from the thermal conductivity one on the crystal quality, the Ge crystallizations were performed using the $0.1 \mu\text{m}$ thick SiO_2 underlayer overcoated with thin Ta_2O_5 ($0.02 \mu\text{m}$ thick) instead of Ta_2O_5 alone. Since the thickness of Ta_2O_5 and W are several tenths of that of SiO_2 , the heat flow of channel (3) is mainly governed by the $0.1\text{-}\mu\text{m}$ SiO_2 underlayer.

Figure 5 compares etch pit patterns of Ge grown on the $\text{Ta}_2\text{O}_5(0.02 \mu\text{m})/\text{SiO}_2(0.1 \mu\text{m})$, $\text{SiO}_2(0.1 \mu\text{m})$, and $\text{W}(0.03 \mu\text{m})/\text{SiO}_2(0.1 \mu\text{m})$ underlayers. Etching was performed using CP-4 etchant. Etch pits reflect the crystallinity at the Ge/ Ta_2O_5 interface since most of the defects, mainly dislocations, originated at the interface will thread through the Ge film and terminate on the surface if the layer is thin. The etch pit densities (EPD) of Ge on Ta_2O_5 , SiO_2 , and W were, respectively, $3 \times 10^6 \text{ cm}^{-2}$, $1 \times 10^7 \text{ cm}^{-2}$, and $1 \times 10^6 \text{ cm}^{-2}$. These results clearly demonstrate that the significant parameter for ensuring high crystal quality is not thermal conductivity but wettability.

§4 Conclusion

Ta_2O_5 was found to be a suitable material for use as an underlying insulator in Ge crystal film growth and that single-crystal GaAs/Ge layers grown on Ta_2O_5 -

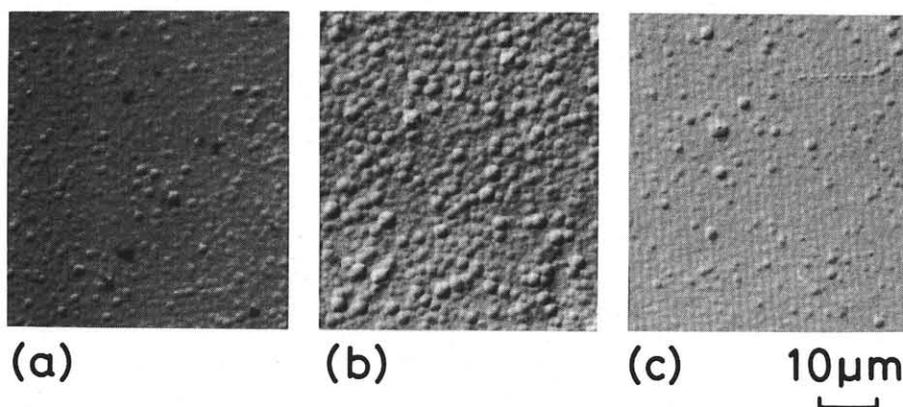


Fig. 5 Etch pit morphology of Ge surfaces grown on Ta_2O_5 (a), SiO_2 (b), and W (c).

coated Si substrates exhibit high-quality characteristics. The results were discussed from the standpoint of the residual stress in Ge, the latent heat liberation and the degree of wettability obtained. The Ge wettability on an insulator was confirmed to significantly influence the crystallinity as well as the large-area Ge crystallization.

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References

- 1) Y. Shinoda, T. Nishioka and Y. Ohmachi : Jpn. J. Appl. Phys. **22**(1983) L450.
- 2) Y. Ohmachi, Y. Shinoda, and T. Nishioka : *International Electron Devices Meeting Technical Digest*, Boston 1983, 315.
- 3) T. Nishioka, Y. Shinoda and Y. Ohmachi : J. Appl. Phys. **56**(1984) 336.
- 4) M. Takai, T. Tanigawa, K. Gamo and S. Namba : Jpn. J. Appl. Phys. **23**(1984) L357.
- 5) T. Nishioka, Y. Shinoda and Y. Ohmachi : J. Appl. Phys. **57**(1985) 276.
- 6) R. L. Chapman, J. C. C. Fan, H. J. Zeiger and R. P. Gale : Appl. Phys. Lett. **37**(1980) 292.
- 7) Y. Ohmachi, T. Nishioka and Y. Shinoda : Electron. Lett. **19**(1983) 274.
- 8) Y. Shinoda and Y. Ohmachi : Proc. MRS, vol. 56, *Layered Structure and Epitaxy*, Boston 1985, J. M. Gibson, G. C. Osbourn, R. M. Tromp eds. (North

Holland, New York, 1986).

- 9) B. Chalmers : *Principles of Solidification* (Robert E. Krieger Publishing Company, Malabar, Florida, 1982).
- 10) J. A. Knapp : J. Appl. Phys. **58**(1985) 2584.