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# Heteroepitaxy of GaAs on Si with Intermediate Layers of Evaporated Ge and Recrystallized Ge-on-Insulator (GOI)

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GaAs layers have been epitaxially grown on Si substrates with intermediate layers of Ge. Epitaxial Ge was obtained either directly on Si using evaporation or laterally on oxide/nitride coated Si using zone-melt recrystallization. X-ray, RBS, PL and TEM studies revealed excellent crystalline quality, suggesting that Ge is a good crystalline match for GaAs. Preliminary studies, based on chemical and electrical characterization, reveal that Si diffusion in GaAs could be as much responsible as Ge for causing an increased level of carrier concentration in GaAs. These studies collectively suggest that Ge intermediate layers could be epitaxially and chemically useful in matching GaAs to Si, although a detailed investigation is still required. Ge could be an essential intermediate layer for GaAs on oxide/nitride coated Si.

## 1. INTRODUCTION

Hybrid crystal films of GaAs on Si substrates are extremely attractive for monolithic integration of GaAs-based devices and/or Si-based devices on common substrates of Si. Such hybridization offers applications in high-speed electronics, opto-electronic integration and chip-to-chip optical communication. It brings forth a complementary utilization of the compound material and silicon material systems that have been independently developed to a high degree of utility and sophistication. To date, GaAs MESFET devices,[1] bipolar devices,[2] lasers,[3] LEDs[4] and the integration thereof on Si, have been reported.[5]

From a materials point of view, the issues of lattice mismatch, thermal mismatch and chemical inter-diffusion have to be properly addressed. In the case of GaAs on Si, the lattice mismatch is 4% and the thermal mismatch, 55%. The possibility of interatomic diffusion has also been reported.[5] In order to overcome one or more or these issues, researchers have pursued GaAs on Si by several different approaches. They include: (1) direct epitaxy of GaAs on Si,[2,6] (2) use of intermediate layers such as Ge or superlattices,[4,7] and (3) use of insulating layers such as silicon-dioxide or calcium fluoride on Si.[8] The Ge in the second case, for example, is epitaxially well-matched to GaAs with lattice-mismatch of only 0.08%. The 4% mismatch between Ge and Si can be more easily accomodated than that between GaAs and Si. Thermally, too, GaAs is better-matched to Ge (2%) than to Si (55%). The use of insulating layers in the third case is geared to three-dimensional (3-D) circuit construction by providing dielectric isolation. Related efforts for 3-D VLSI integration have been pursued in SOI (Si-on-insulator) technology.[9]

This paper describes several approaches that we have taken to attain GaAs on Si, particularly using intermediate layers of Ge, either directly on Si or indirectly on insulator-coated Si. In the former, Ge was evaporated on Si and in the latter Ge was recrystallized over insulator-coated Si. Various characterization results were used to determine the structural, chemical and electrical properties of these materials.

## 2. EXPERIMENTAL

Ge on Si. Ge was grown on Si using an electron-beam evaporator which has background pressure of $10^{-6}$ - $10^{-7}$ torr. Silicon substrates were initially dipped in buffered HF solution before loading. After loading, silicon wafers were heated to $900^{\circ}$C for 10 minutes to remove residual oxides. Epitaxial Ge was grown at temperatures between $350^{\circ}$C - $700^{\circ}$C. The growth rate varied between 2-70Å/sec depending on the growth temperature. Silicon substrates were either p-type in (100) or (111) orientations.

Ge-on-insulator (GOI) Si wafers of (100) or (111) orientation were first thermally oxidized up to 0.5 mm thickness. The thermal oxide was then photolithographically patterned in such a way as to form oxide blocks separated by grooves. The size of island blocks ranged from 5 x 5 microns up to 500 x 400 microns. The grooves were 10 microns wide. Ge films were then deposited on the oxide-patterned Si either at room temperature or at an elevated temperature between 450 - 650$^{0}$C. At room temperature, Ge was deposited in a non-crystalline state whether on the oxide blocks or on the grooves. At an elevated temperature, Ge on the groove was grown in single crystals, as seeded from the Si, while Ge on the oxide grew in micro-polycrystals. Thin (300-500 Å) tungsten layers were finally deposited on Ge in order to keep Ge from evaporating during recrystallization. Ge on oxide was recrystallized using an Argon ion laser or a strip-heater. In both cases, the GOI samples were heated to 750$^{0}$C during recrystallition. Scan speed in the laser crystallization was between 1-5 mm/sec, and in the strip-heater crystallization, 1-2 cm/sec. Laser beams were focused into an oval line having 1.5 mm x 50 micron aspect ratio, delivering 4-6 watts of cw power. Strip-heaters were normally heated up to 1600$^{0}$C at a distance of 1mm from the Ge film.[10b]

GaAs Deposition. Epitaxial GaAs layers were deposited on the Ge-coated Si and GOI materials using MOCVD or MBE. MOCVD GaAs was grown at atmospheric pressure and MBE GaAs was grown at $10^{-10}$ torr. The growth temperature was varied between 600$^{0}$and 675$^{0}$C. In the case of GOI, tungsten capping layers were chemically etched off prior to GaAs deposition, using a mixture of $K_3Fe(CN)_6$ and NaOH in water. Films were grown with thickness between .5 μm and 5.0 μm.

## 3. RESULTS AND DISCUSSION

GaAs on Ge/Si. The morphology of GaAs and of evaporated Ge epi-layers (typically 1-2 microns thick) on (100) Si substrates were macroscopically mirror-smooth and appeared free of cracks. Microscopically, the Ge surface also appeared smooth, but GaAs showed antiphase domain structures. X-ray diffraction consistently showed excellent crystallinity for both GaAs and Ge layers. The RBS (Rutherford Back Scattering) of a 1.1 μm thick GaAs film shows $\chi$ min approaching 3.5% and that of 1.5 μm Ge, to 3.6% (Fig. 1). Cross-sectional TEM (Transmission Electron Microscopy) shows remarkably low defect density at the Ge surface in spite of the high density misfit dislocations at the Ge/Si junction. Crude defect-counting, based on chemical etching, shows that the defect density in the Ge decreases toward the surface with an exponential trend.[10a] Interestingly enough, the residual dislocations in the Ge upper layer do not necessarily thread into the GaAs layer (Fig. 2). The good crystalline quality of GaAs was further evidenced by PL (photoluminescence) measurements, which revealed a peak at 852 nm (1.455 ev) with FWHM of 14 meV. X-ray rocking curve results also revealed good crystalline quality for GaAs on Ge, showing line width of about 200 arc seconds. These results collectively indicate that GaAs is well-matched to Ge.

An unresolved concern for GaAs on Ge is chemical interdiffusion between the two layers. The concern for chemical interdiffusion is greater for GaAs on Ge than for GaAs-on-Si, as the Ge diffusivity in GaAs is known to be higher than the Si diffusivity in GaAs. EDX (Energy Dispersed X-ray), SIMS, Auger and spreading resistance measurements have shown evidences that both Ge and Si diffuse into GaAs. The degree of diffusion between Si and Ge, however, seems to be an unresolved issue. In our findings, by Au Schottky barrier characterization, there exists evidence that Ge diffuses less than Si.[11] More study is required for a better understanding of Ge and Si diffusion behavior in GaAs.

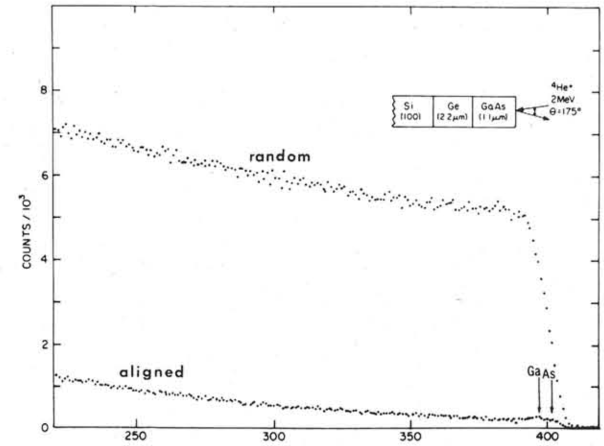


Fig. 1. Rutherford Backscattering Spectra of MOCVD GaAs layer grown on Ge-coated Si, showing $\chi$min of about 3.5%.

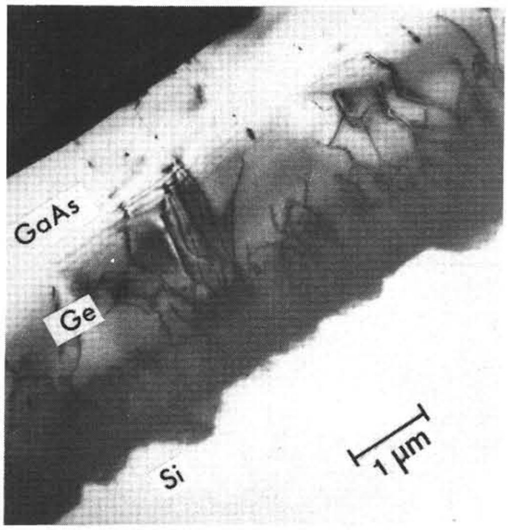


Fig. 2. Cross-sectional TEM of MOCVD GaAs on Si with epitaxial Ge intermediate layer.

GaAs on GOI. Ge-on-insulator (GOI) offers an advantage of forming GaAs epi-layers on dielectrically isolated Si substrates. The potential of such a structure lie in the application of high-speed and high-density electronics and three-dimensional (3-D) circuit construction. In our study of seeded crystallization, single crystals of Ge have been obtained up to 50μm x 400 μm and 160 μm x 160 μm (Fig.3). Subboundaries, that are commonly observed in SOI, were very rarely observed in GOI due to different crystallization mechanism.[12] Cross-sectional TEM shows that the defect density at the Ge/insulator interface is far lower than that at the Ge/Si interface.[10b] The quality and morphology of subsequent GaAs crystals depend strongly on the characterisitcs and orientation of recrystallized Ge. In the (100) seeded GOI, indication of anti-phase domain structure was evident (Fig. 4). In unseeded GOI, where the Ge was recrystallized in mixed orientation, GaAs morphology showed both anti-phase domain structures and single domain structures, depending on the orientation of individual Ge crystallites. The morphological variation results from the different manner in which Ga and As stick to the Ge lattice at various orientations. Micro-beam x-ray or Raman analysis is underway to correlate the morphological variation of GaAs to the orientation of respective Ge crystals.

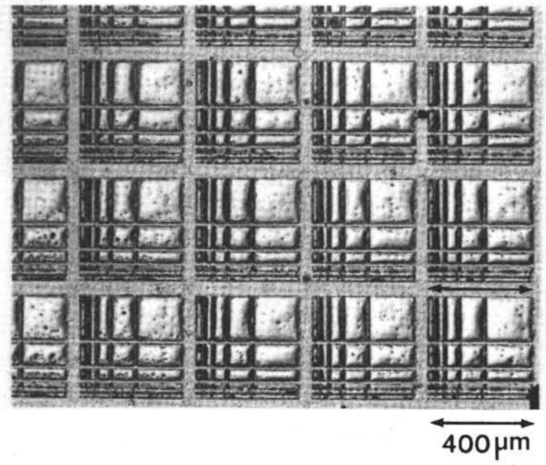


Fig. 3. An array of crystalline Ge-on-insulator (GOI) island patches attained with zone-melt recrystallization technique. Laser scanning was from right to left.

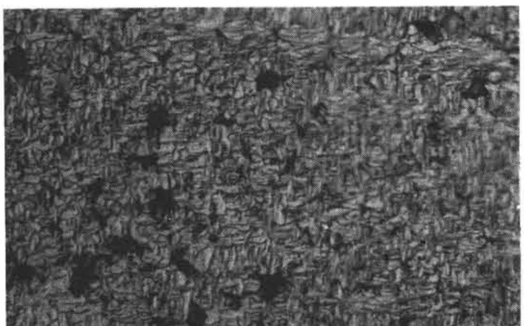


Fig. 4. Morphology of MOCVD GaAs on (100) GOI. Bi-directional granular feature suggests anti-phase domain structure.

## 4. SUMMARY AND CONCLUSION

Epitaxial GaAs layers have been grown on Si substrates with intermediate layers of Ge. Ge layers were grown either directly on Si by evaporation or laterally on oxide/nitride-coated Si using beam-recrystallization. X-ray, photo-luminescence, RBS and TEM studies show excellent crystallinity for GaAs on Ge-evaporated Si. The crystalline quality of GOI, as studied by RBS, appears somewhat inferior to the Ge grown directly on Si. TEM cross-section shows, however, that the defect density at the Ge/insulator interface is much lower than that at the Ge/Si interface. From a structural view point Ge appears to be a good match for GaAs. From a chemical point of view, however, the question of the Ge and Si interdiffusion in GaAs is still an unresolved issue. In our preliminary studies, based on electrical and chemical characterization, Ge diffusion appears less severe than that of Si, suggesting that Ge could be favored, both epitaxially and chemically, as an intermediate layer. For GaAs epitaxy on oxide/nitride-coated Si, recrystallized Ge would be essential.

## 5. ACKNOWLEDGEMENT

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11. E.Y. Chan, M.A. Awal and E.H. Lee (Unpublished results).

12. E.H. Lee and M.A. Awal (Unpublished results).