

Silicon-Germanium-Carbon Alloys Extending Si Based Heterostructure Engineering

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SiGe epitaxial growth on Si has been of interest for a number of years. In this work we consider the addition of C into both Si and SiGe epitaxial material. We have used solid and gas sources for the C and produce high crystalline quality material from both approaches. We also demonstrate strain symmetrised short period superlattice structures grown on (100) Si with high Ge compositions ranging from 20% up to 60% Ge.

Introduction

In the past ten years epitaxial SiGe material has proved itself to be of high crystalline quality and has provided impressive results in bandgap engineered device structures. The addition of Ge onto the Si lattice provides compressive strain which reduces the bandgap by lifting the degeneracy of the conduction band and lowering the 4 fold degenerate conduction valley. When C is added to Si the grown layer is under tensile strain, this will again lift the degeneracy and this time the 2 fold degenerate conduction band is expected to be lowered, thus giving a net reduction in the bandgap for strained $\text{Si}_{1-y}\text{C}_y$ material.

For cubic, i.e. relaxed $\text{Si}_{1-y}\text{C}_y$ material the band gap should increase towards the value of 2.2eV for the 50% alloy, β -SiC. As the band structures of Si and β -SiC are quantitatively similar, with the conduction band minima positioned near the X(100) zone edge there should be no question of an L-X crossover, as in the SiGe case, this has been considered in ref1.

Growth

Growth of the $\text{Si}_{1-y}\text{C}_y$ alloy is more limited than the SiGe case as the C is not miscible with the Si material, (it has a solubility of $<10^{-6}$ at 1400°C). At higher temperatures the more stable carbide phases are formed however if the growth temperature is reduced such that the growth can be kinetically stabilized then

the random alloy may be deposited. The second important aspect of C is that the lattice mismatch to Si is high 52% (for diamond). However, as in this work it is the induced strain that is important, only low compositions of $\text{Si}_{1-y}\text{C}_y$ alloy are required. For example, 1% of C gives approximately the same magnitude of strain as 11% of Ge in the Si matrix.

In this work we have used two differing approaches to the deposition of C into the Si matrix.

The first method is to use a solid elemental carbon (graphite) filament which is heated to in excess of 3000°C in order to sublime C atoms from the filament. This has been described previously², and provides a flux of C atoms to the Si surface.

The second method that we have employed is to flow acetylene into the MBE chamber during deposition of Si. To achieve this we have used a standard VG MBE system and attached gas input lines and turbo pumping. The base pressure of the system remains in the 10^{-10} torr regime and rises to 5×10^{-9} torr during the growth of the Si layers. To deposit the $\text{Si}_{1-y}\text{C}_y$ layers acetylene is allowed to flow through the system increasing the pressure to 2×10^{-7} torr. The growth temperatures used are between 500°C and 600°C and the composition of the $\text{Si}_{1-y}\text{C}_y$ layer is controlled by the Si flux rate, typically 1 to 10 nm/min.

The high epitaxial quality of the $\text{Si}_{1-y}\text{C}_y$ grown with the solid C source has been previously demonstrated², The quality of the $\text{Si}_{1-y}\text{C}_y$ grown

utilizing the gas source can be seen from the lack of additional broadening of the X-ray diffraction rocking curve obtainable from a 1.5% C 1000A $\text{Si}_{1-y}\text{C}_y$ layer, Fig 1. This layer is close to the expected critical thickness for a layer grown at this temperature, 525°C^3 and the same composition layer grown at the higher temperature of 600°C was found to be relaxed.

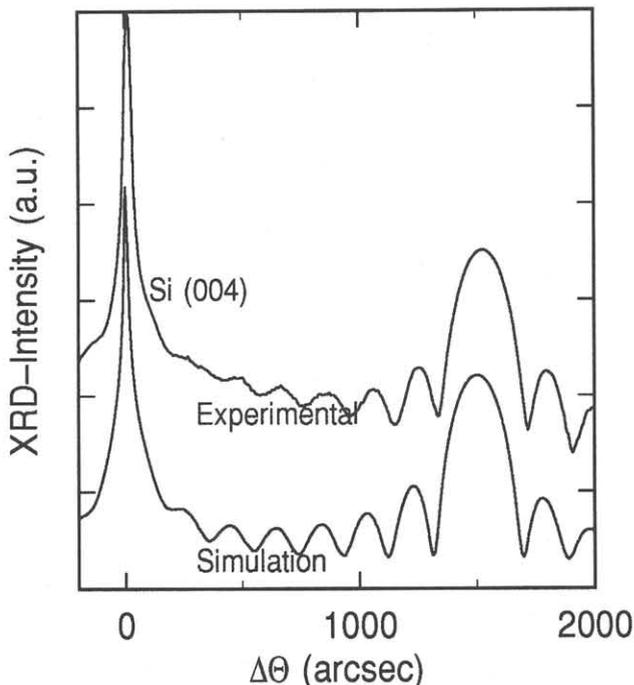


Fig 1 Experimental and simulation x-ray diffraction rocking curves (004) of a 100 ± 5 nm $\text{Si}_{1-y}\text{C}_y$ with $y=0.015$.

Superlattice Deposition

Both systems also allow the growth of Ge from a solid Ge source and utilizing the solid C source we have produced short period (13 Angstrom) symmetrically strained superlattices. The superlattices that we have grown consist of alternating $\text{Si}_{1-y}\text{C}_y$ and SiGe layers. The structures were grown at temperatures ranging from 525°C for low composition alloys to 475°C for the higher composition alloys, in addition to this Sb was deposited on the structure prior to the superlattice growth to provide surfactant action during deposition in order to prevent Ge segregation. A number of structures were grown with nominal compositions shown in table 1.

Table 1

Sample	$\text{Si}_{1-y}\text{C}_y$	$\text{Si}_{1-x}\text{Ge}_x$	Number Of Periods
1	0.5nm $y=0.03$	0.8nm $x=0.2$	140
2	0.8nm $y=0.03$	0.5nm $x=0.4$	140
3	0.8nm $y=0.04$	0.5nm $x=0.55$	140
4	0.8nm $y=0.08$	0.5nm $x=1.0$	28

The material quality of the superlattice structures degrades as the C and Ge compositions are increased. This is due to difficulties in producing high composition $\text{Si}_{1-y}\text{C}_y$ alloys without the introduction of SiC precipitates. However even at compositions as high as 55% Ge we are still able to produce sufficiently high quality material to give clear rocking curves in x-ray diffraction.

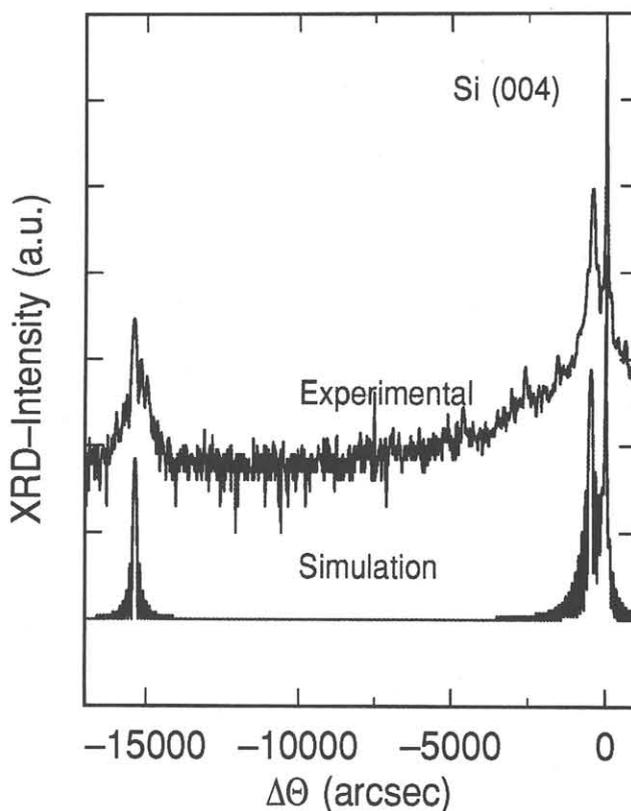


Fig 2 Experimental and simulation x-ray diffraction rocking curves (004) of sample #3, a short period superlattice with $\text{Si}_{1-y}\text{C}_y$ and SiGe layers.

Fig 2 shows the (004) double crystal rocking curve for sample no 3. This curve clearly shows the

"-1" superlattice peak at -15500 arcsec, from the superlattice peak separation the average period can be accurately found to be 1.30 ± 0.02 nm. In addition near the "-1" peak it can be seen that some of the diffracted signal has been shifted into the nearby pendellosung peaks, this is due to some period dispersion within the superlattice structure⁴. The "0" order superlattice peak at -450 arcsec shows that there is a small amount, 1.9×10^{-3} , of unequalized strain remaining in the superlattice. However, this is considerably less than the expected 9.2×10^{-3} that would be seen without the presence of the C.

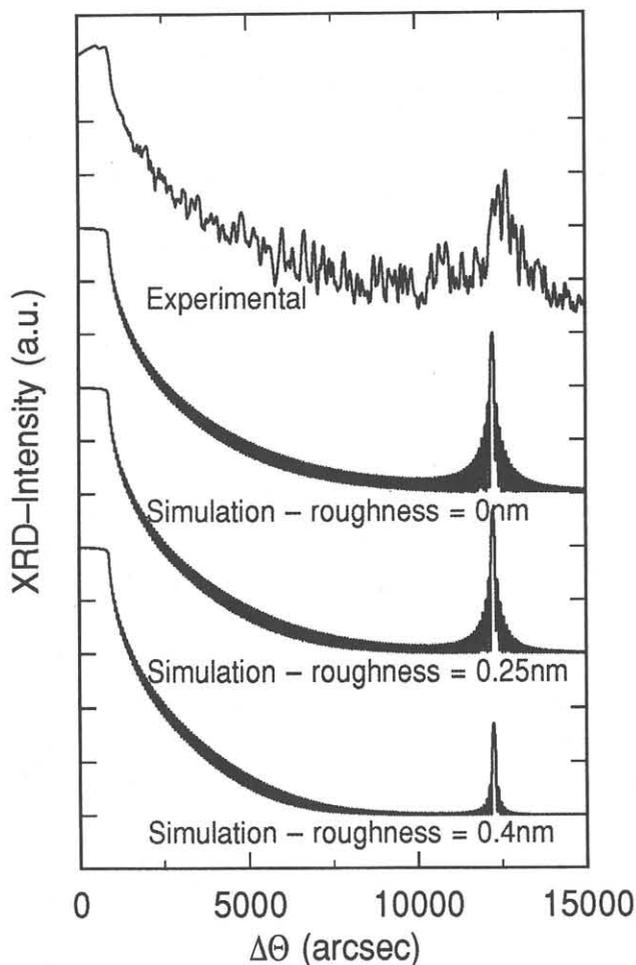


Fig 3 Experimental and simulation reflectivity curves of sample #3 showing the first superlattice reflectivity peak, at 12000 arcsec.

In order to determine the interface quality within the superlattice structure X-ray reflectivity was used which is sensitive to both short range and long range roughness in the interfaces. Fig 3 shows the

curve obtained from sample #3 along with three simulations demonstrating how the intensity in the reflectivity peak decreases with increasing interface roughness.

In the reflectivity curve intensity, has again been transferred into subsidiary pendellosung peaks from the main superlattice peak. However, in this measurement it is the total integrated intensity around the Superlattice peak which is important. We find that this integrated intensity is such that it can be matched by simulations with interface roughness values lower than 0.3 nm. At roughness greater than this the peak intensity is seen to rapidly fall off. At roughness values of less than 0.25 nm the interface roughness can be dominated by the random nature of the SiGe and SiC alloys and thus roughness values less than this can only be considered meaningful for superlattices consisting of elemental layers such as a Si/Ge superlattice.

Conclusions

In this work we have demonstrated high quality growth of $\text{Si}_{1-y}\text{C}_y$ material using both solid and gas sources for the C. The growth of short period strain symmetrised superlattices has also been presented with a high degree of control on the period of the structures and high quality interfaces.

Acknowledgments

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