Growth Phenomena of Si/$Si_{1-x-y}Ge_xC_y$ Epilayers and Superlattices

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Heteroepitaxial growth allows the reduction of the dimensionality of a carrier system along the growth direction by exploiting carrier confinement at heterointerfaces. A further reduction to 1D and 0D systems requires in addition either lateral structuring or a self-organized growth scheme. We investigate both approaches in the $Si_{1-x-y}Ge_xC_y$ heterosystem by using epitaxial growth on pre-patterned substrates and a novel route to quantum dots with mono-modal size distribution.

1. Introduction

The investigation of low-dimensional structures becomes increasingly relevant as critical dimensions of commercial devices reach the nanometer range. Presently, devices with gate lengths of 65 nm are in large scale production (130 nm technology node), and the SIA roadmaps predict critical dimensions of 9 nm for 2016. This top-down-approach by down-scaling of existing technologies has in recent years been supplemented by attempts to use self-assembling growth phenomena for the fabrication of 1D and 0D quantum systems. Here we report on two such attempts in the $Si_{1-x-y}Ge_xC_y$ material system, namely the epitaxial overgrowth of pre-patterned substrates, and the growth of SiC quantum dots. This material system is of special interest because of its compatibility with standard Si technologies.

2. Morphological Development of Si Wire Templates During Annealing and Overgrowth

The exploitation of structured substrate templates is an attractive option both in connection with self-organization growth modes, and for improved defect control of relaxed SiGe buffer layers. On Si(001) substrates we prepared wire structures with periods down to 300 nm by holographic lithography and reactive ion etching. The photoresist and RIE residues were removed wet-chemically, and just before MBE growth a thermal cleaning step was performed *in situ* at 900 – 950 °C. We found an unexpectedly large surface mass transport even at these temperatures, which are significantly below the melting point of Si (1330 °C). Wires of square or a slight trapezoidal cross section develop pronounced {311} facets, concomitant with a significant loss of height. Overgrowth with SiGe superlattices partly reestablish the (001) top facet, which becomes wider with increasing epilayer thickness (Figs. 1, 2). These results have important implications for the shape preservation of structured substrates during annealing and overgrowth.

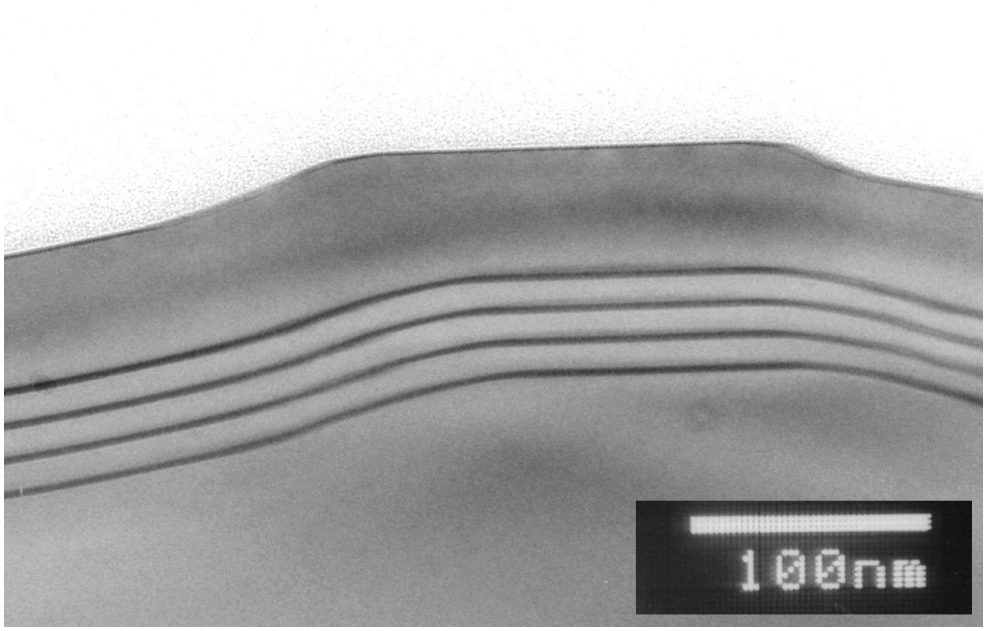

Fig. 1: XTEM image of a Si wire structure overgrown by a Si/SiGe superlattice. Thermal annealing led to substantial mass transport on the Si template that transformed the slightly trapezoidal wire cross sections into flat wires with [311} side facets.

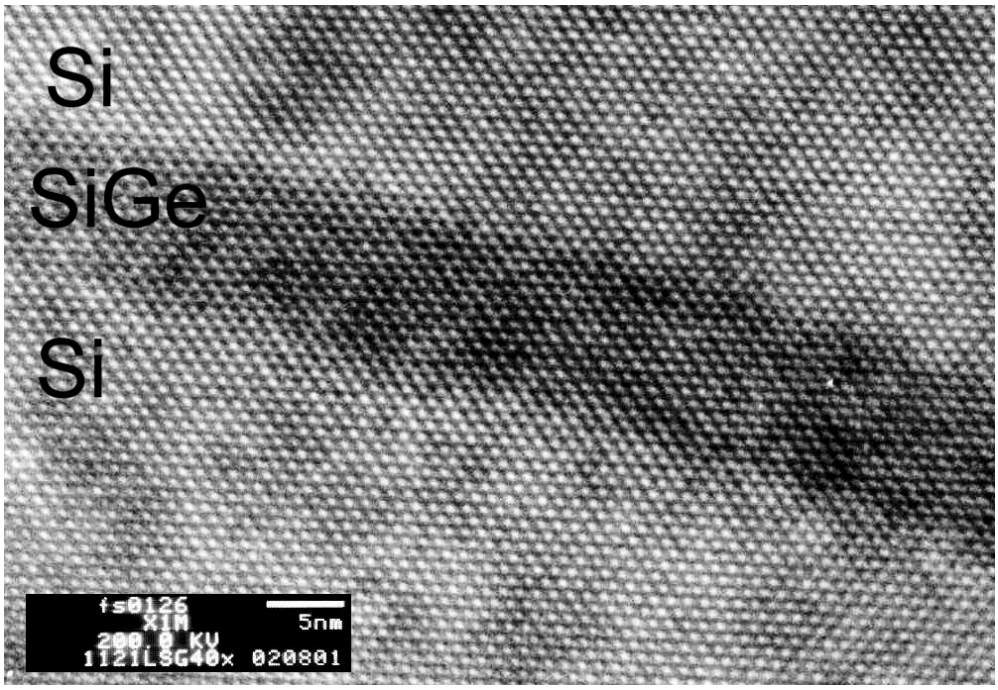

Fig. 2: High resolution XTEM of the superlattice in Fig. 1. The image was taken in a region where the (001) top facet is gradually transformed into a {311} facet that was created by thermal cleaning of the wire-structured substrate.

3. β-SiC Formation

Carbon concentrations exceeding the solid solubility limit of about 10^{17} cm^{-3} lead to β-SiC precipitation near thermal equilibrium. This can be a detrimental effect if it happens, e.g., during processing of high-speed SiGeC heterobipolar transistors (see separate report on FTIR spectroscopy of C-complexes in Si). On the other hand, such β-SiC precipitates may be useful for the creation of quantum dots in Si. For that purpose carbon clusters of well-defined size are incorporated into a Si matrix and subsequently converted into β-SiC by high temperature annealing. Especially attractive appear the use of Fullerens (C_{60}), or of defined fractions of these molecules which became available recently, because they would allow a mono-modal size distribution of the β-SiC clusters. Because of the larger band gap of β-SiC the clusters are not quantum dots themselves, but they can be used as stressors to induce carrier confinement in the surrounding Si matrix or in a near-by SiGe layer.

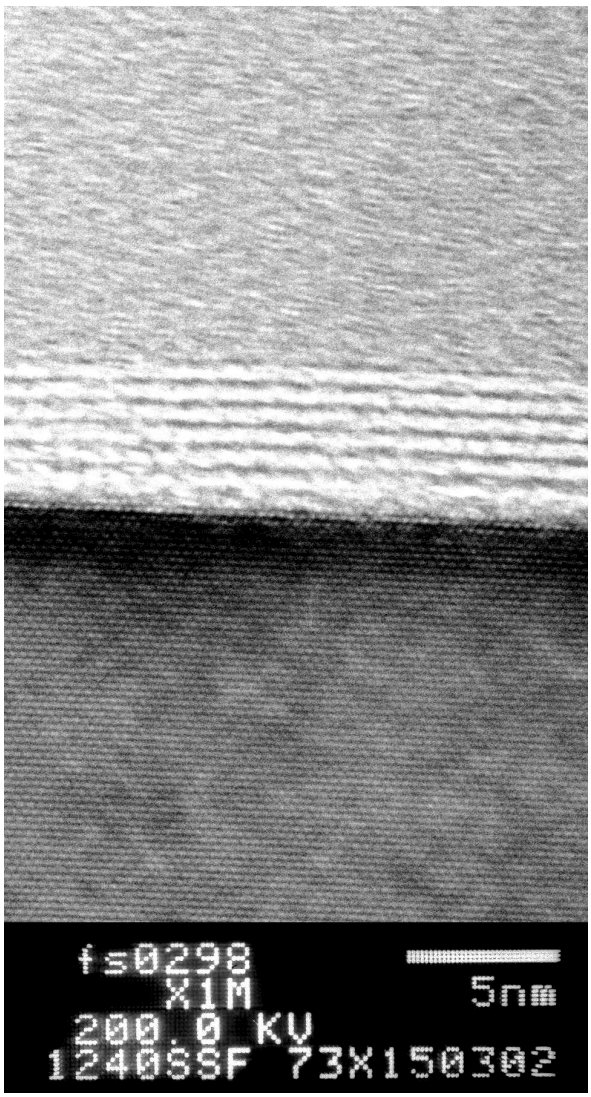

Fig. 3: Layer sequence for the calibration of the C_{60} source. In the XTEM micrograph 7 monolayers of Fullerens can be seen. The lower layer is crystalline Si(001) (point resolution is 0.32 nm), above the Fulleren layer an amorphous Si cap layer has been deposited.

The experiments are performed in a newly commissioned growth chamber for the deposition of Fullerens, which is attached to the our Siva 45 Si-MBE machine. To calibrate the flux of the Fulleren source, relatively thick layers were deposited on a Si substrate at room temperature and subsequently capped by amorphous Si. Figure 3 shows a high resolution XTEM image of such a layer sequence. Seven monolayers of C_{60} on the crystalline Si substrate can be distinguished. Because of the low deposition temperature, the C_{60} layer is polycrystalline. With flux calibration from Fig. 3, submonolayer C_{60} coverages were deposited at 300 K, capped by 5 nm of amorphous Si, annealed at 1200 °C, and finally overgrown by 15 nm of crystalline Si. Figure 4 shows an example of such a layer sequence. SiC clusters are clearly distinguishable through a Moiré pattern that develops when crystalline materials with different lattice constants are contained within the thickness of the TEM specimen. In addition, defective solid phase overgrowth can be seen above one of the SiC particles. The size of the SiC inclusions is on the order of 5 nm, i.e. much larger than expected from the reaction of an individual C_{60} molecule. Obviously, even at the low deposition temperatures employed, clustering of Fullerens must have taken place. Further experiments are required to demonstrate the feasibility of SiC particles created from isolated C_{60} molecules. The aim is to optimize the growth parameters until pseudomorphic β-SiC clusters of identical size and strain fields can be produced.

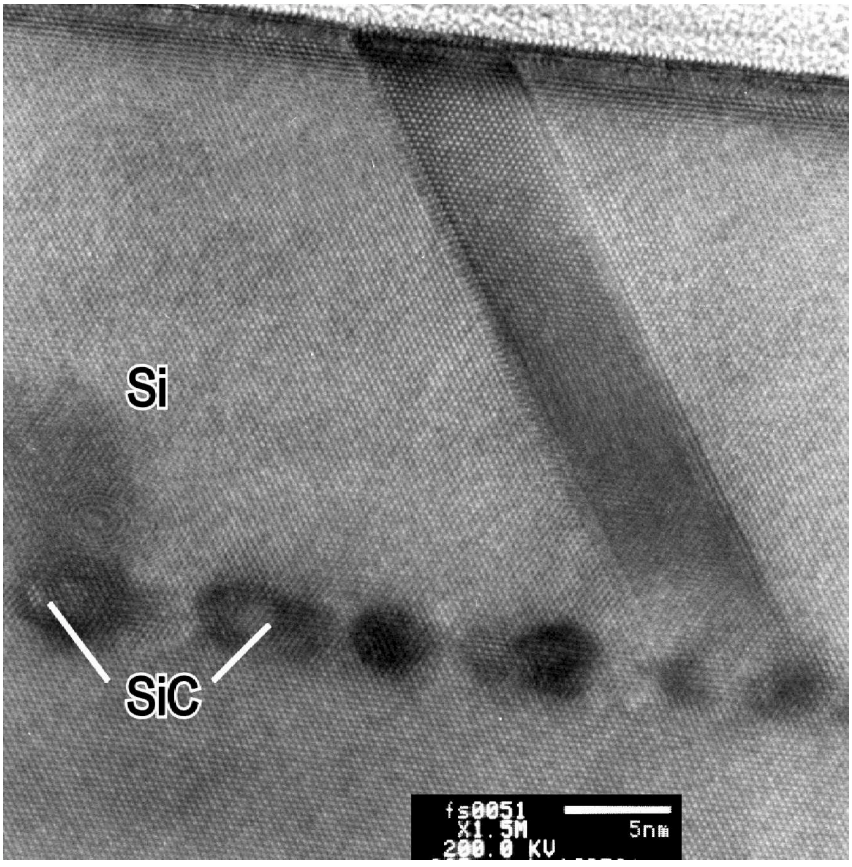

Fig. 4: β-SiC nanocrystals generated by high-temperature annealing of Fulleren clusters that were capped by amorphous Si. The contrast results from lattice distortions and partial dislocations that have formed around the incoherent β-SiC nanocrystals.

4. Conclusions

Two approaches are followed to produce 1D and 0D structures in the $Si_{1-x-y}Ge_xC_y$ heterosystem. In both cases unexpected growth phenomena were encountered, which require further optimization of the growth parameters. The use of Fullerens for the implementation of mono-modal quantum dots appears promising, but requires addition experiments to suppress clustering of the weakly bound C_{60} molecules.

Acknowledgements

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