Fourier Transform Infrared Spectroscopy of β-SiC Precipitation in SiGeC Epilayers

D. Gruber, T. Fromherz, M. Mühlberger, F. Schäffler

Institut für Halbleiter- und Festkörperphysik, Johannes-Kepler-Universität Linz, A-4040 Linz

1. Introduction

The ternary $Si_{1-x-y}Ge_xC_y$ alloy was considered a promising material for band structure engineering of Si-based heterostructures. However, in contrast to the binary $Si_{1-x}Ge_x$ alloys, which are completely miscible, C has a negligible solid solubility in both Si and Ge, and only one stable phase, that of SiC. This makes metastable $Si_{1-x-y}Ge_xC_y$ alloys with useful C concentrations of a few tenths of a percent unstable against the formation of β-SiC precipitates. A typical example is shown in Fig. 1: The high-resolution cross sectional transmission electron micrograph (XTEM) shows incoherent β-SiC precipitates in a single crystalline Si matrix. Since Si and β-SiC differ in their respective lattice constants by about 20%, a Moiré pattern becomes observable at places where relaxed β-SiC precipitates are surrounded by undisturbed Si. The spacing of the Moiré pattern depends on the difference of the two lattice constants, and thus allows an unambiguous identification of β-SiC.

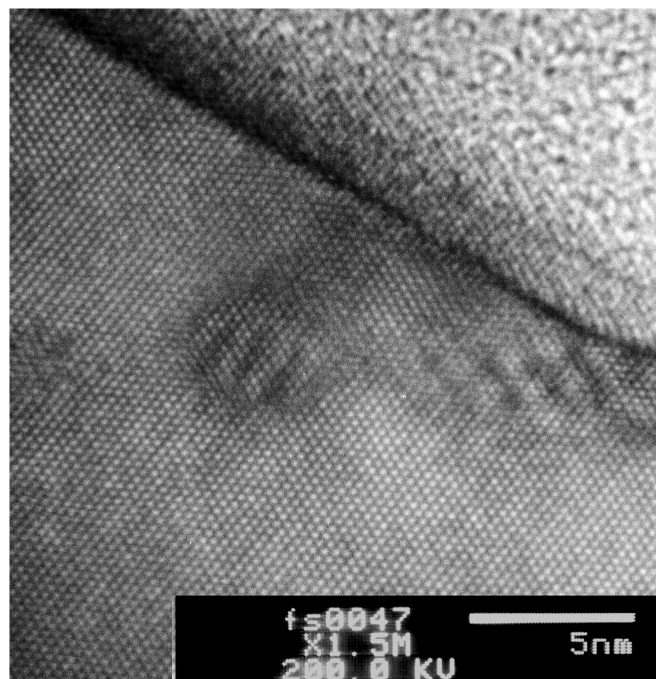

Fig. 1: XTEM micrograph of β-SiC precipitates in a Si matrix. Individual Si [111} lattice planes with a spacing of 3Å are resolved. The β-SiC precipitates lead to a Moiré pattern because of their 20% smaller lattice constant.

β-SiC precipitation restricts the potential use of $Si_{1-x-y}Ge_xC_y$ alloys to applications that can either be kept far from thermal equilibrium or require very small amounts of carbon. The most interesting of these applications is the exploitation of substitutional carbon (C_S) for the suppression of transient enhanced diffusion (TED) of Boron in Si/SiGe:C heterobipolar transistors. But even though the required C concentrations are reasonably low (0.2 at.%), high temperature annealing steps are unavoidable during standard Si technology. It is therefore necessary to optimize the layer parameters and thermal budgets.

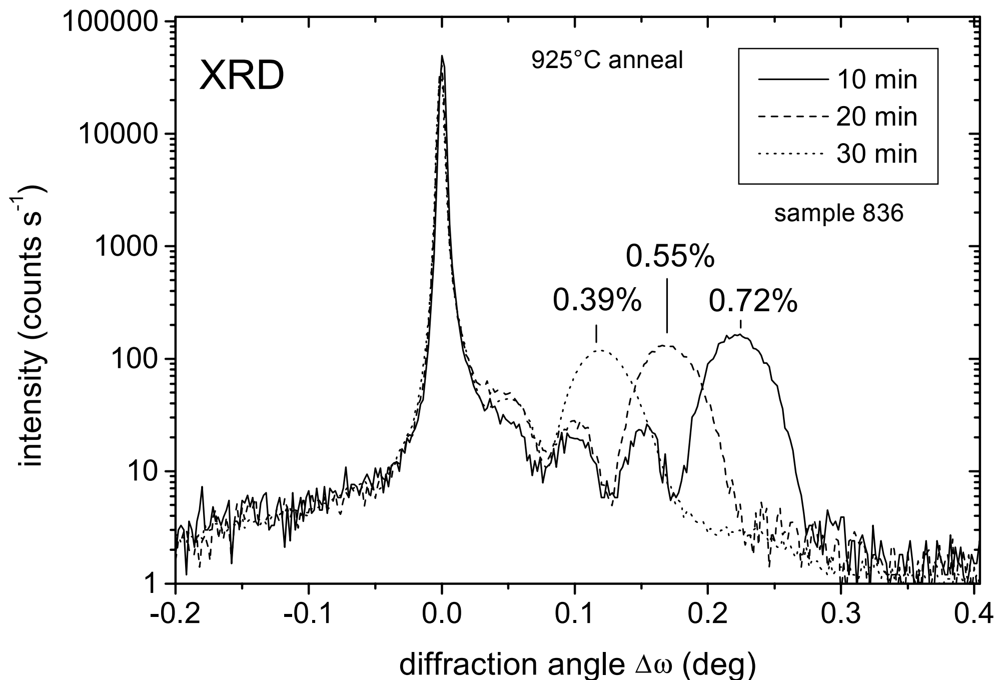

Fig. 2: X-ray rocking curves of $Si_{1-y}C_y$ films that underwent annealing at 925 °C for increasing periods of time. The (smaller) $Si_{1-y}C_y$ peak moves toward the (dominant) substrate peak with prolonged annealing time, indicating gradual relaxation of the film stress. The curves are labeled with their remaining substitutional carbon concentration y_{eff} that has to be compared to y = 1% of the as-grown sample.

2. Experimental

Based on the standard AIST procedure for the characterization of C_S in bulk Si, we exploit the local vibration modes of C to identify the local chemical environment [1]. This gives access not only to the concentration of C_S, but also to pseudomorphic and incoherent β-SiC precipitates. Problems are the small absolute concentrations of either type of C bonds in the thin epilayers under study, and the presence of a Si phonon mode that overlaps the relevant frequency range of the local modes. It is therefore essential to achieve high sensitivity and accurate subtraction of the bulk signal. These aims were achieved by employing Fourier Transform Infrared Spectroscopy (FTIR), and thickness corrections for the reference bulk sample with an accuracy of a few µm. The latter was achieved by a first FTIR reference measurement with high resolution (cm^{-1}), which

gives access to the sample thickness via the thickness interference fringes of the plan-parallel, one-sided polished substrates. For the subsequent measurement of the local carbon vibration modes the resolution was then lowered to 4 cm^{-1} to suppress the thickness fringes.

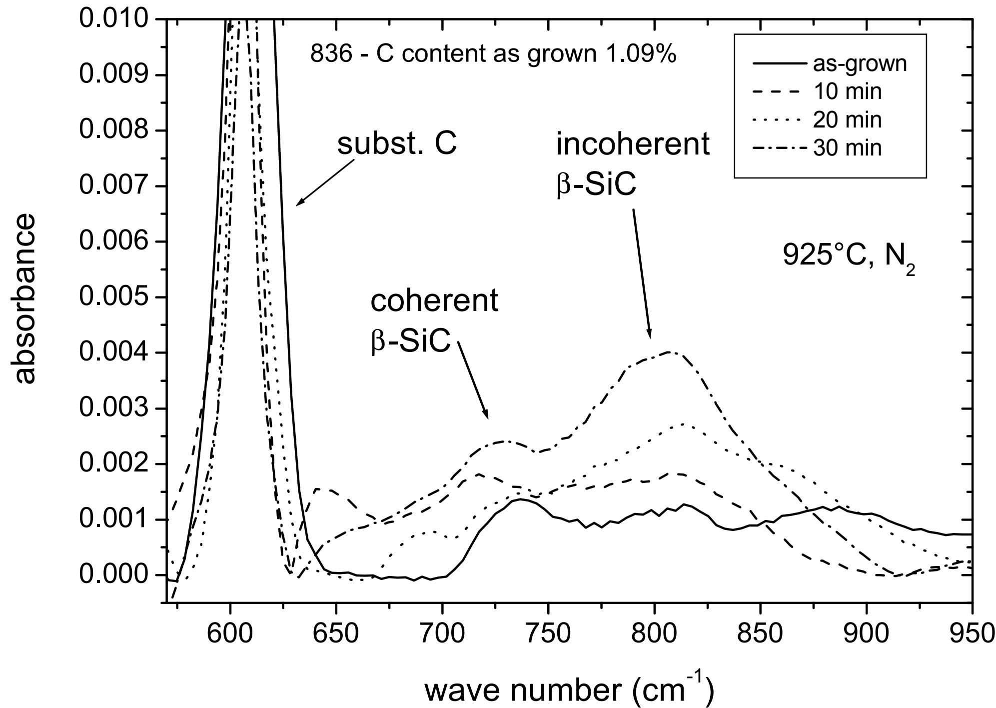

Fig. 3: FTIR spectra of the sample in Fig. 2 in the frequency range of the carbon-related local vibration modes. With increasing annealing time more and more carbon moves from substitutional into SiC sites.

3. Results

Figures 2 and 3 show typical results of 100 nm thick $Si_{0.99}C_{0.01}$ films annealed at process temperatures of 925 °C for various times. The x-ray rocking curves in Fig. 2 reveal a substantial amount of film relaxation, with <40% of the originally present C remaining at substitutional sites. This can directly been followed in the attenuation of the local C_s mode at 608 cm^{-1} in the FTIR spectra of Fig. 3. Simultaneously, the signals at 750 and 820 cm^{-1} gain intensity, indicating that coherent, and incoherent β-SiC, respectively, have formed, which are the main sources of strain relaxation in these films.

To study the time scale for complete film relaxation, similar films were annealed at 1000 °C for extended periods of time. Under these conditions we found that after 240 min the films were completely relaxed: The local mode of substitutional C has then vanished, and most of the C has formed incoherent β-SiC precipitates (Fig. 4). Correspondingly, no $Si_{1-y}C_y$-related signal can be observed in the x-ray rocking curves.

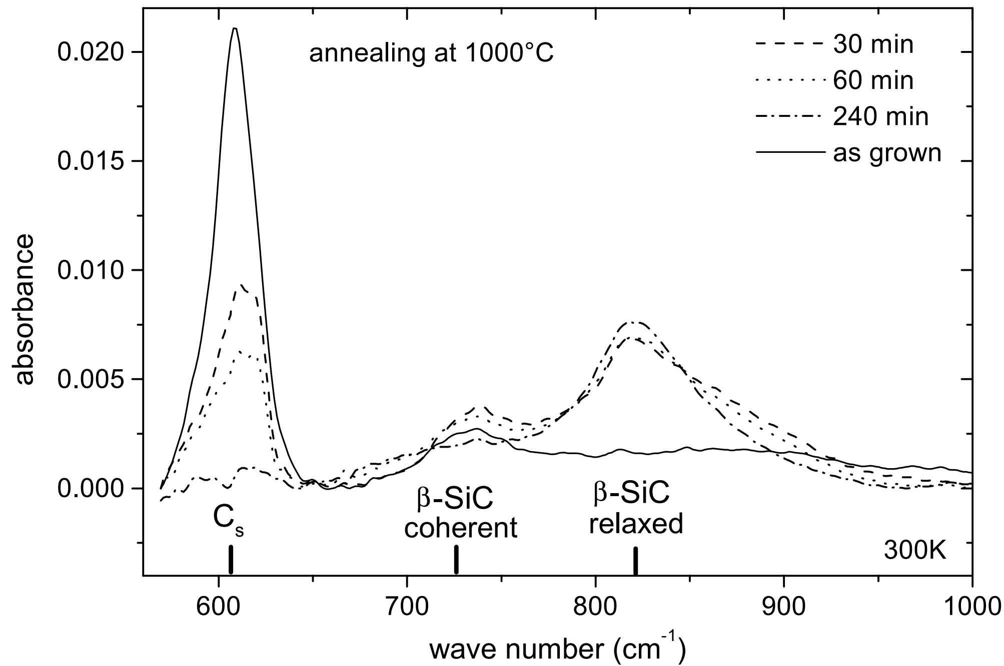

Fig. 4: Same as Fig. 3 but annealing at 1000 °C for extended periods of time. Note that substitutional carbon has completely disappeared after 240 min at 1000 °C.

4. Conclusion

The results have important implications for the application of $Si_{1-x-y}Ge_xC_y$ films. Typical processing temperatures during standard Si technology are comparable to our experimental range, with 925 °C being a rather low limit for the activation of implanted contact regions. However, processing times are significantly shorter than in our oven anneals, typically on the order of 1 min (rapid thermal processing [RTA]). Our experiments show that the formation of β-SiC precipitates is a rather slow process, provided the C concentrations are kept at low enough levels. Hence, even 1000 °C RTA steps may be acceptable, if processing steps are kept low enough. However, generally both the C concentration and the thermal budget of the process should be kept as low as possible. In any case, monitoring of the complete device processing with respect to β-SiC precipitation is important. FTIR is the technique of choice with respect to sensitivity and selectivity of different carbon environments. Of course, electrical measurements of e.g. the generation/recombination behavior are required in addition.

References

[1] D.Gruber et al., *Mat. Sci. Eng.* **B89**, 97 (2001)