Strained Silicon Above and Below Ge Islands

A. Hesse[1], J. Stangl[1], V. Holý[1], G. Bauer[1], U. Denker[2], O.G. Schmidt[2]

[1]Institute for Semiconductor Physics, Univ. Linz, Austria
[2]Max-Planck-Institute, Stuttgart, Germany

We present a method to realize strained Si without graded SiGe layers. By capping self-organized grown Ge islands at sufficiently low temperatures with Si, above and below Ge-dome shaped islands in-plane strain values of about 0.48% are achieved in Si. These high values of tensile in-plane strain are quite important for confining electrons in Si. The structural properties of the capped islands are almost identical to those of uncapped SiGe islands grown under the same conditions.

Introduction

Recently strained Si has found a lot of interest because of the fact that higher electron mobilities as compared to conventional MOS structures can be obtained. Usually relaxed graded SiGe buffers are used to provide the biaxial tensile strain in the subsequently deposited Si layers. However, the strain values that can be achieved using this approach are limited. Furthermore, threading dislocations from the graded buffer layer penetrate through the active strained Si layer. We investigated another method to realize strained Si, which avoids graded SiGe layers and has the advantage that the active strained Si layer is dislocation free. The time to grow Ge islands is essentially shorter than the one used for the graded buffer layer growth. By capping self-organized grown Ge islands at sufficiently low temperatures with Si, above and below Ge-dome shaped islands in-plane strain values of about 0.48% are achieved in Si. Low temperatures can suppress the usually observed changes in shape, composition and strain [1]. However, the optical and electrical properties can deteriorate with decreasing growth temperatures [2]. Therefore, an optimum between sample quality and structural properties has to be found.

Experimental

Three island samples have been grown by solid source molecular beam epitaxy on Si (001) wafers. After the deposition of a Si buffer layer, 5 monolayers of Ge were deposited at a growth temperature of 630 °C, forming dome-shaped islands. The islands were capped with about 150 nm of Si at different temperatures: for sample A the cap layer was grown at 630 °C, as the islands, whereas for samples B and C the growth temperature was lowered to 540 °C and 460 °C, respectively. In order to investigate the Ge distribution, high-resolution x-ray diffraction experiments were performed. Reciprocal space maps (RSMs) were recorded in a coplanar setup around the asymmetrical (224) and (404) Bragg reflections. Figure 1(a)–(d) shows several measured intensity distributions. Panels (a)–(c) show the RSM around the (224) Bragg reflection of sample A, B, and C, respectively. Panel (d) shows additionally the (404) map of sample C. The intensity distributions in Figs. 1(a)–(c) are quite different. For sample A, a maximum elongated along Q_z but narrow along Q_x is observed very close to the truncation rod. This indicates that the SiGe islands are flat and wide and that the strain *with respect to* *the substrate* $\varepsilon_{||} = (a_{||}-a_{Si})/a_{Si}$ is small. On the contrary, for samples B and C peaks wider along Q_x but narrower along Q_z are observed at a larger distance from the truncation rod, corresponding to higher more strained islands with smaller base, especially for sample C.

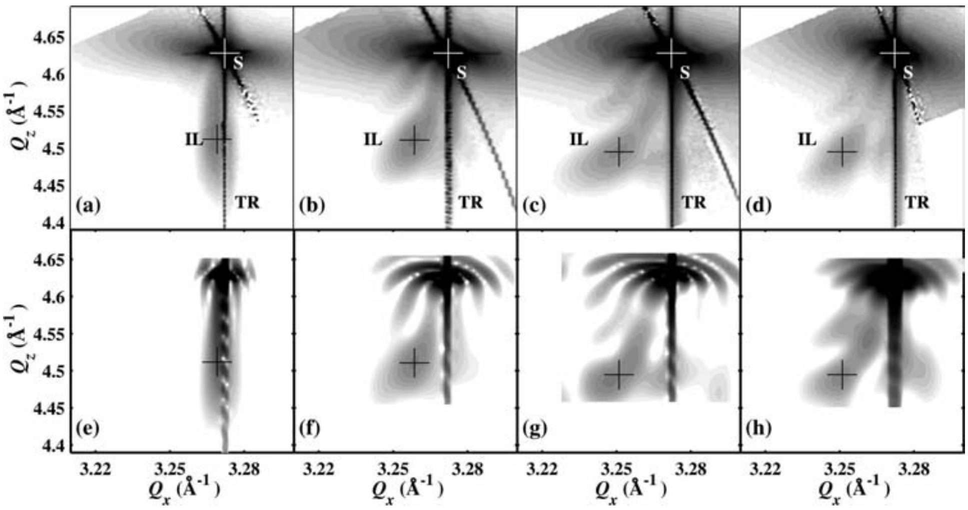

Fig. 1: (a) Measured RSM of sample A around the (224) Bragg reflection of Si. Beside the substrate peak labelled "S" and the crystal truncation rod labelled "TR", diffuse scattering from the buried SiGe islands labelled "IL" is clearly visible. (b) and (c) (224) measured RSMs of samples B and C, respectively. (d) RSM around the (404) reflection of sample C, with Q_x divided by √8/4 for comparison with the (224) RSM. (e),(f), and (g) Simulations of the (224) reflection for samples A, B, C using a parabolic shape. Simulations for sample C using a pyramidal shape are shown as well as (h). 8 contour levels per decade are shown in the RSMs between 10^{-8} and $10^{-5.5}$ relative to the substrate intensity. Crosses denote the position of the maximum scattered intensity.

Figure 1(d) shows the map of sample C recorded around the (404) reflection, i.e., in an azimuth in between the (224) and (2-24) maps. The Q_x-axis in the plot has been rescaled by a factor √8/4. Hence the coordinates along Q_x and Q_z correspond to those in the (224) maps. Obviously, the intensity distribution from the SiGe islands in Fig. 1(c) and Fig. 1(d) shows only small differences.

Results

For a quantitative analysis of the x-ray data, we performed a simulation of the diffuse x-ray scattering pattern. Starting from a model of the island shape and the Ge distribution, the strain fields in and around the islands are calculated using an analytical approach. In accordance with our x-ray diffraction data and investigations using AFM of uncapped islands at comparable samples, we assume an approximately rotationally symmetric shape of the islands. The results for samples A, B, and C are shown in Fig. 1 (e)–(g), respectively. A perfectly rotationally symmetric shape is certainly an idealization. Therefore, we performed simulations not only with a rotationally parabolic shape, but also with the shape of a truncated pyramid, with a square base oriented along <110> directions. Figure 1(g), (h) shows the simulations around the (224) reciprocal lattice point for sample C for both types of shape, with a linear Ge profile optimized for each shape, i.e., with the best correspondence of the *peak position* with the experiment. Again, different assumptions on the shape give slightly different results in the Ge distribution, but within our confidence interval of ± 0.05. It is obvious that the simulated *peak shape* of the diffuse intensity distribution does not perfectly match the experiment (see Fig. 1(c)) in either case, but rather the latter is in between the two simulations. Therefore we conclude that the actual shape of the buried islands is similar to pyramidal islands, but with rounded corners. As the differences in the results are not significant, as far as Ge content and strain values are concerned, we used the values obtained from the parabolic model.

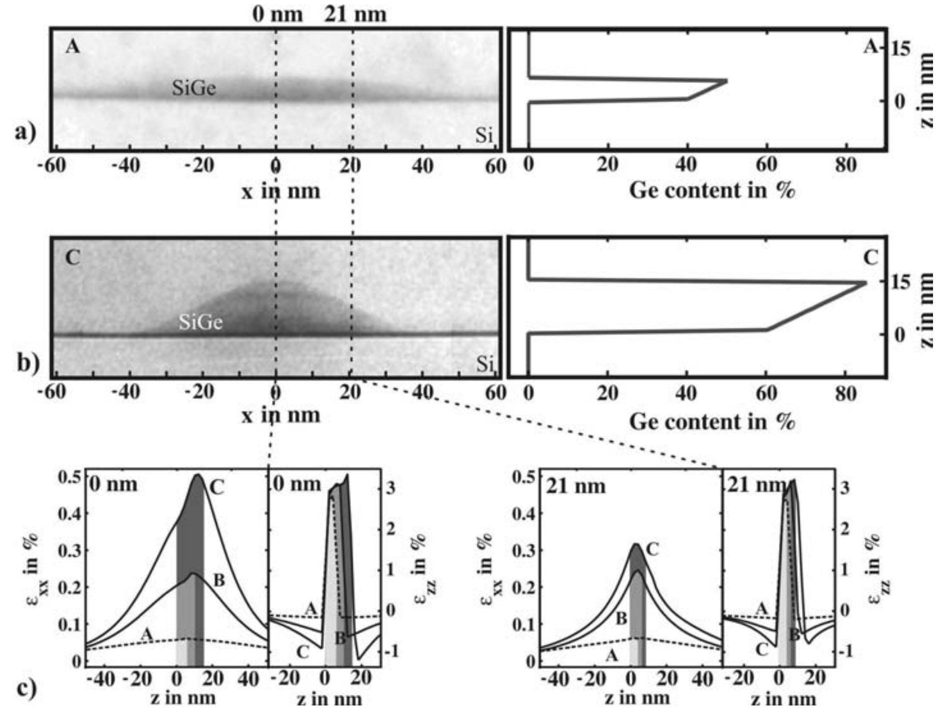

Fig. 2: (a) Cross-sectional transmission electron micrograph of sample A together with Ge composition gradient along height z in the center of the island. (b) as (a) but for sample C. (c) strain tensor components ε_{xx} and ε_{zz} as a function of height z through the center of the island (0 nm) and along a vertical line laterally shifted by 21 nm towards the edge. Note the appreciable amount of in-plane strain above and below the buried island in the tensily strained Si and its drastic decease with increasing Si capping temperature. The z-coordinate=0 in all drawings corresponds to the bottom of the islands. The respective heights of the islands are illustrated by shaded areas.

The results of our analysis are summarized in Fig. 2. For sample A capped at 630 °C we obtain a base width of the islands of about 100 nm and a height of about 6.6 nm. For the in-plane strain ε_{xx} values around 0.06 % without a significant variation within the island. The Ge content varies from 0.4 at the base to 0.5 at the apex of the island, as shown in Fig. 2(a). These values are almost identical to those obtained in a previous study on buried islands [3]. For samples B and C capped at 540 °C and 460 °C, respectively, however, the properties are considerably different: for the lowest capping temperature, the base width and height of the islands are evaluated to be about 70 nm and 15 nm, respectively. The structural properties of the islands capped at low temperatures are almost identical to those of uncapped SiGe islands grown under the same conditions [4]. The prevention of the flattening leads to a much higher lateral strain ε_{xx} in Fig. 2(c) for sample C, i.e., 0.38 % at the base and 0.48 % at the apex. The much larger lateral strain values are a consequence of the higher Ge content within the islands in sample C: We obtain a variation from x=0.6 at the base to 0.85 at the apex (see Fig. 2(b)), actually close to the properties of uncapped islands grown under the same conditions. For sample B we obtained for the islands values between those of sample A and B, i.e., a base width of 84 nm, a height of 10.5 nm and a Ge content variation between x=0.4 (base) and 0.8 (top). In Fig. 2(c), these strain values ε_{xx} and ε_{zz} are shown for a vertical cross-section along the center of the island and in addition along a vertical line shifted laterally by 21 nm towards the edge of the islands. Our study clearly shows that the shape, strain and Ge distribution of capped islands depends sensitively on the growth temperature used for Si capping. For the lowest capping temperature of 460 °C, the structural properties of the Ge islands are nearly preserved. We would like to point out that the capping temperature has also a drastic influence on the strain status of tensily strained Si up to about 50 nm, i.e., 3 to 4 times the island height, above and below the Ge island. For the lowest capping temperature, the maximum in-plane strain in the Si matrix immediately above the island is as high as 0.48 %. These high values of tensile in-plane strain are quite important for confining electrons in Si.

Conclusion

We have investigated a series of SiGe islands grown on Si(001) and capped with Si at temperatures 630 °C, 540 °C, and 460 °C. The change of shape, strain, and Ge distribution observed at high capping temperatures of 630 °C can be drastically suppressed by lowering the capping temperature to 460 °C. The structural properties of the islands capped at low temperatures are almost identical to those of uncapped SiGe islands grown under the same conditions.

References

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