Strain and Composition of SiGe Islands on Si (001)

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We have investigated the strain and composition distribution in uncapped SiGe islands on Si (001) by x-ray diffraction. In order to be sensitive to the dot layer at the sample surface, and at the same time being able to measure in-plane strain and strain in growth direction, we utilized a scattering geometry at grazing incidence angles, but with high exit angles. The measured intensity distribution is compared to simulations based on the strain distribution calculated by the finite element method. It turns out that, although pure Ge has been deposited during island growth by molecular beam epitaxy, the Ge composition varies from 0.5 at the island base to 1.0 at the top of the islands. The elastic relaxation reaches only about 50% even at the island top.

1. Introduction

Recent years have seen a series of studies shedding light on the formation of so-called self-organized nanostructures during semiconductor heteroepitaxy. They are formed due to a growth instability in strained heterostructures. After a certain critical thickness of deposited material, in our case Ge on Si, three-dimensional islands form on top of a two-dimensional layer, the so-called wetting layer (WL). These islands can elastically relax and hence reduce their strain energy, which is the driving force of their formation. The main advantage of such islands as compared to nanostructures fabricated, e.g., by etching, is the high areal density and the virtually complete absence of defects [1].

However, it is difficult to control the size, strain and composition of self-organized structures because these quantities depend very sensitively on the growth conditions (substrate temperature, adatom flux, etc.). Transmission electron microscopy (TEM) has been used to investigate the strain distribution within such islands [2], [3]. Recently, also the Ge and Si distributions in uncapped SiGe islands have been investigated using TEM, showing that islands formed during the deposition of pure Ge onto a Si surface are alloyed [4]. On the other hand, TEM investigations on Ge islands grown by chemical vapor deposition of 11 ML of Ge at 600 °C have been interpreted as not giving evidence for significant alloying [5].

X-ray diffraction (XRD) techniques have also been applied to tackle the question of strain and composition [6], [7]. In principle, XRD is the method of choice to measure strains, and often the strain state can be directly related to a composition. This is a standard technique for the investigation of, e.g., SiGe buffer layers with graded composition. However, for objects as small as self-organized islands, the correct spatial localization of a certain strain state is an ambitious task.

2. Experimental

Our investigations focus on a sample (S1183B4) with free-standing SiGe islands grown by MBE on [001]-oriented Si. After growth of a Si buffer layer and a buried SiGe island layer, a layer of Ge islands at the surface was formed by the deposition of 6 ML of Ge. The growth temperature was 600 °C. Here we are interested solely in the surface islands; the buried islands have no influence on the scattered signal due to the low incidence angle $\alpha_i = 0.15°$ (below the critical angle $\alpha_c \approx 0.22°$). With AFM two types of islands have been detected on the sample surface, larger ones with a base diameter of about 175 nm and a height of 30 to 70 nm, but with a low density of about 2×10^7 cm^{-2}, and smaller ones with a high density of about 4×10^9 cm^{-2}, and a height and base diameter of about 13 nm and 110 nm, respectively. Here, we consider only the smaller islands, and neglect the scattering from the larger islands because of their low density.

In order to distinguish between material composition and strain state, we measure not only the in-plane lattice parameter, as in grazing incidence diffraction studies, but also the lattice parameter in growth direction. This can be achieved by measuring reciprocal space maps (RSMs) with the momentum transfer component along growth direction $Q_z > 0$, as illustrated in Fig. 1(a) and (b). RSMs have been recorded around the (202) reciprocal lattice point (RLP) of Si, which is inaccessible in the conventional coplanar geometry at a wavelength of 1.55 Å, but can be accessed by rotating the scattering plane around the scattering vector $\mathbf{Q}$, out of the plane of the RSM, as is shown in Fig. 1(c). With this setup, it is possible to keep the incidence angle α_i and hence the penetration depth constant at a value below ac for the entire RSM, in order to be sensitive to the dot layer at the sample surface.
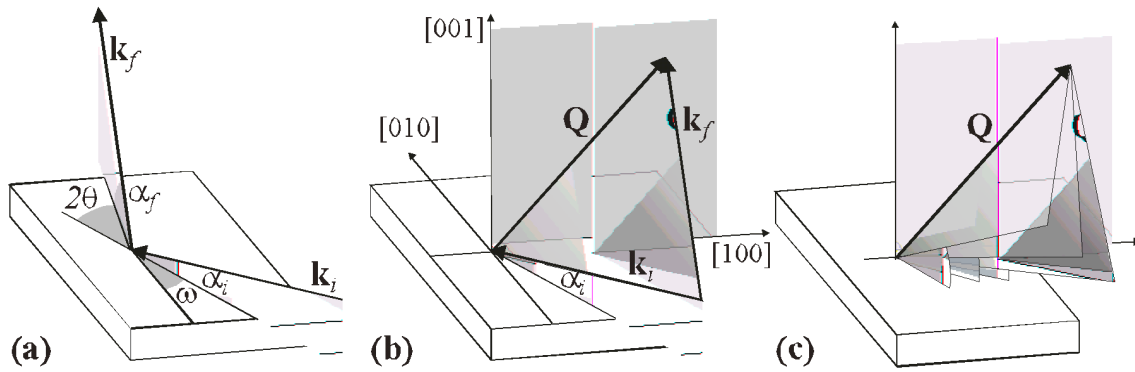

Fig. 1:   Illustration of the scattering geometry in real space (a) and reciprocal space (b). (c) Tuning of the incidence angle by rotating the scattering plane around the scattering vector $\mathbf{Q}$.

For the determination of the Ge distribution within the islands, we use kind of a "fitting" procedure: we start with an assumption on the Ge distribution and calculate the strain distribution using the finite element method (FEM). With this result the XRD pattern is calculated, and compared to the experimental result. Repeating the procedure while varying Ge distribution and island shape until a good correspondence between experiment and simulation is reached, we are able to establish the distributions of Ge content and strain within the islands. We assumed islands with the shape of a rotational parabo-

loid. With the FEM data, RMSs have been calculated using a kinematic scattering theory, and as well assuming a cylindrical symmetry.

Figure 2(a) shows the measured intensity distribution. Taking simply the peak maximum position Q_{max} and calculating the lattice parameters via the relation $a_{\parallel,\perp} = 2\pi/Q_{x,z}$, we would obtain values for the composition $x_{Ge} = 0.73$ and for the in-plane strain with respect to the substrate $\varepsilon_{\parallel} = (a_{\parallel} - a_{Si})/a_{Si} = 0.011$. The results of our simulations are shown in Fig. 2(b) – (d). Using a constant composition of the SiGe islands, no good correspondence with the experiment can be obtained: assuming an island with the constant composition of $x_{Ge} = 0.73$, the simulation yields a peak at a different position than the measurement, at the correct value of Q_z, but at a too large value of Q_x (Fig. 2(c)).
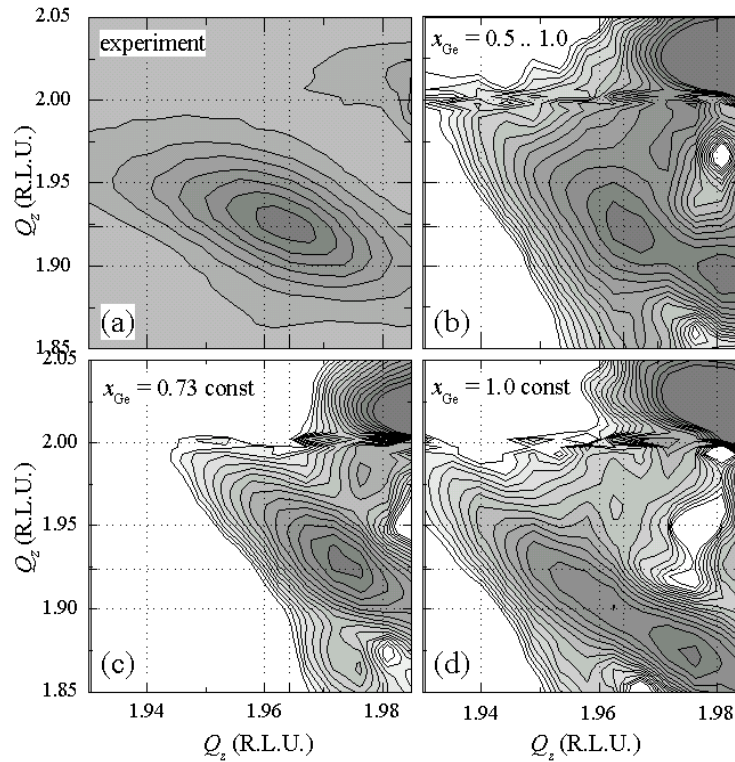

Fig. 2: (a) Reciprocal space map around the (202) Bragg reflection. (b) – (d) Simulations with different assumptions on the Ge distribution within the islands.

The reason for this difference is quite clear: the simple evaluation of the peak position assumes an island with homogeneous composition and homogeneous strain. As the island is grown pseudomorphically on the Si substrate, but relaxed towards the top, at least the latter cannot be true. We varied the composition of the island to obtain a smaller Q_x of the peak maximum. At $x_{Ge} = 1.0$ (Fig. 2(d)), the peak position is almost correct along Q_x, but now Q_z is too small. Hence it is clear that assuming a constant composition, no agreement with the experiment can be achieved. Thus we varied the Ge composition distribution within the island from a value $x_{Ge,1}$ at the base to a value $x_{Ge,2}$ at the top. Within the islands, the Ge content was assumed to be constant laterally, and only a vertical profile, either linear, or increasing like $z^{1/2}$ (i.e., the Ge content increases faster at the bottom of the island than on its top) or z^2 (Ge content increasing faster at the

top of the island than on its base), was assumed. We found the best correspondence between simulation and experiment for a faster increase of the Ge content at the base of the islands. Figure 2(b) shows the calculated RSM for a Ge distribution which reproduces the peak position best, with a maximum content of $x_{Ge,2} = 1.0$ at the top of the island, and $x_{Ge,1} = 0.5$. In contrast to, e.g., InAs Islands on GaAs [7], the maximum in-plane strain at the top of the islands reaches only about 0.02, i.e., the dot is only about 50% relaxed even at the top.

3. Conclusion

In summary, from our study it is evident that albeit pure Ge is deposited during MBE growth, the uncapped islands are alloyed, and the Ge content varies from about $x = 0.5$ at the base to $x = 1.0$ at the top (these particular values will depend sensitively on the growth parameters). We believe that the reduced elastic energy of an interdiffused island, [8] as compared to an island of pure Ge, is the main driving force for the alloying.

Acknowledgements

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