Strain and composition of SiGe islands on Si (001)

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We have investigated the strain and composition distribution in free-standing 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, a Ge composition gradient within the islands exists.

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 α_i=0.15° (below the critical angle α_c≈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 $Q_z > 0$. The measurements have been performed at TROÏKA II beamline at the ESRF (Dr. D. Smilgies). The 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 **Q**, out of the plane of the RSM, as is shown in Fig. 1. With this setup, it is possible to keep the incidence angle α_i and hence the penetration depth constant at a value below α_c for the entire RSM, in order to be sensitive to the dot layer at the sample surface.

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

Figure 2(a) shows the measured intensity distribution. Taking simply the peak maximum position $\mathbf{Q}_{max}$ 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)].

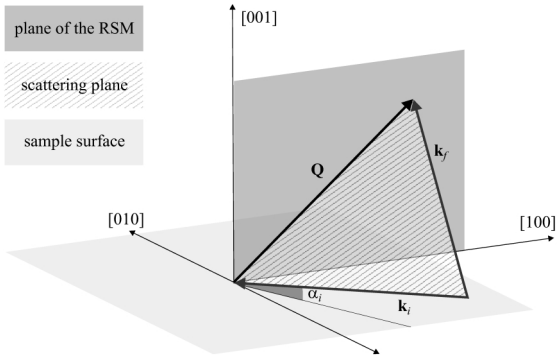

Fig. 1: Sketch of the scattering geometry:

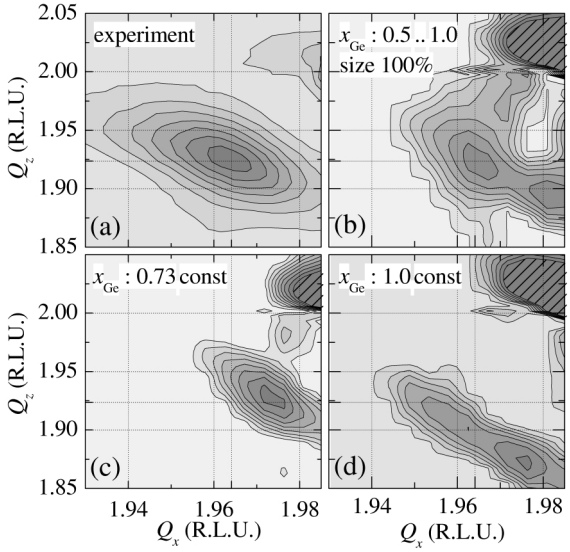

Fig. 2: (a) Reciprocal space map around the (202) Bragg reflection. (b)-(d) simulations with different assumptions on the Ge distribution within the islands.

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 $z^{½}$ (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 $x_{Ge,1} = 0.5$. We believe that the reduced elastic energy of an interdiffused island, as compared to an island of pure Ge, is the main driving force for the alloying.

PUBLICATIONS*:* J. Stangl, A. Daniel, V. Holý, T. Roch, G. Bauer, I Kegel, T.H. Metzger, T. Wiebach, O.G. Schmidt, K. Eberl, Appl. Phys. Lett., submitted.

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