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Colloque VIIIA : Surface et interface

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Relaxation and Intermixing Behavior in SiGe Islands Grown on Prepatterned Si(001)

We investigated the lattice relaxation and composition of Ge islands on nominal Si(001) and pre-patterned substrates grown at identical conditions. Reciprocal space mapping is combined with anomalous diffraction and atomic force microscopy. This combined method allows for the determination of thermodynamic potentials as elastic energy and the entropy of mixing and their corresponding volume average and thus the energy stored per atom in one island.

The samples where transferred after growth under N_2 atmosphere to the UHV-diffractometre on BM32 at the ESRF in Grenoble. A selected region of the sample had been patterned prior to growth in order to obtain highly homogeneous and ordered islands [1,2]. Reciprocal space maps taken on the unpatented and the patterned region of the substrate are shown in Fig. 1 together with AFM images as insets. Size oscillations witness in both cases very narrow size distribution. Furthermore, the higher lattice relaxtion for the patterned case in (b) is clearly visible. Islands on the nominal sample part have their main lattice relaxation at lattice parameters around 0.546 nm whereas for the patterned part, the lattice-parameters are streched over a longer area in reciprocal space, showing a maximum at about 0.551 nm.

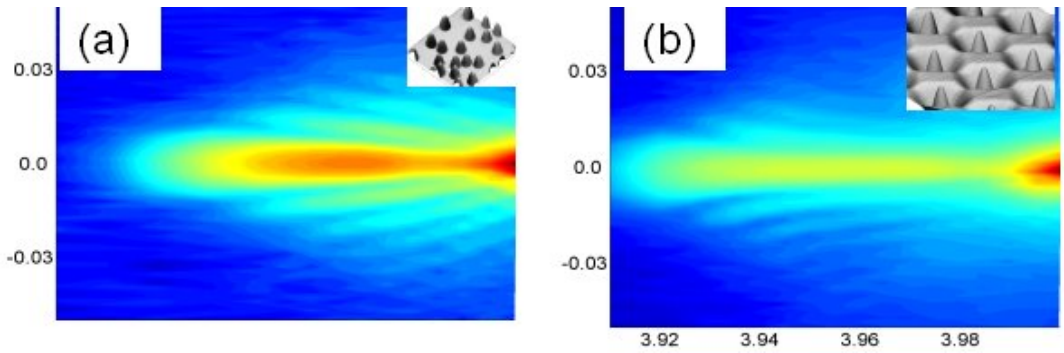

Fig 1 (a) : Reciprocal space map around the 400 Bragg reflection for the SK-grown sample on the nominal part. The inset shows an AFM image of this region. (b) :The same region of reciprocal space as in (a) but for the Ge-islands grown on the patterned part.

This 1 % difference in lattice parameter can have several origins. (1) The concentration gradient might be more important in the islands on the patterned part with a maximum Ge concentration that exceeds the one present in the islands grown on the nominal part. (2) The island growth on the patterned part leads to higher relaxation. In order to to determine the

Ge content inside the islands, anomalous x-ray scattering was applied [3,4]. It yields similar concentrations for both island types and thus a remarkable difference in the stored elastic energy inside the islands.

From the composition of the $SiGe$ alloy, the elastic parameters ν (poisson ratio), μ (shear modulus) and the corresponding equilibrium lattice parameter a_{eq} where calculated. Assuming linear elasticity, the elastic energy was calculated and a mean value per atom was averaged over the whole island volume. It turns out, that for the islands grown on the patterned part, the elastic enery is about 50 % lower then on the nominal part. Being grown under identical conditions and showing similar compositions this indicates that strain cannot act as a driving force for interdiffusion.

In order to shed light on this modified Stranski Krastanov growth on patterned substrates, we performed Monte Carlo simulations of both growth types and compared them with Monte Carlo fits, taking into account the x-ray data of Ge-content as a function of lattice parameter. It is shown that the combination of these method together with the boundary conditions supplied by experimental data as size, mean compostion and composition as a function of lattice parameter, allows making a statement about the proximity to thermodynamic equilibrium of such a structure.

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