Ordering of Strained Ge Islands on Prepatterned Si(001) Substrates: Morphological Evolution and Nucleation Mechanisms

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Introduction

The spontaneous formation of 3D islands during epitaxial growth of lattice-mismatched heteromaterials (Stranski-Krastanov [SK] growth) has become the most important self-organization mechanism for the fabrication of coherently embedded nanostructures. However, the randomness of island nucleation, and the broad distribution of their size severely restrict the application potential of this approach: Most electronic and spintronic device applications require the individual addressability of such nanostructures, and thus a means for the precise control of their nucleation sites.

We realized perfectly ordered SiGe and Ge islands in two (2D) and three dimensions (3D) by providing preferential nucleation sites through nanostructuring for the SK growth mode [1]. The islands nucleate preferentially at the bottom of reactively ion etched pits, which assume the shape of truncated inverted pyramids, after overgrowth with a thin Si buffer layer. This nucleation site is at first sight rather surprising, because it appears to be the least favorable site for strain relaxation within the pit template. To gain a better understanding of the mechanisms that lead to the preferential nucleation of the Ge dots there, we studied the very early stages of Ge coverage in detail [2].

Experimental

The samples were grown by solid source molecular beam epitaxy (MBE) in a Riber SIVA 45 reactor. Pit-patterned templates on Si(001) substrates were obtained by electron beam lithography and reactive ion etching (RIE) in SF_6. The pits form a regular two-dimensional grid ordered along two orthogonal <110> directions with a periodicity between 260 and 380 nm. After etching, the samples were chemically cleaned to remove RIE deposits and residues from the e-beam resist. Immediately before introduction into the MBE reactor the samples were treated in diluted HF to create a hydrogen terminated surface that stabilizes the nanostructures against transient enhanced diffusion during the following *in situ* thermal treatment at 900°C for 5 minutes. Since we wanted to characterize the very early stages of ordered Stranski-Krastanov growth on prepatterned substrates, we employed growth conditions that were optimized for this purpose over the last few years. MBE growth always commenced with a 100 nm thick Si buffer layer that was grown at a rate of 0.5 Å/s while ramping the substrate temperature from 450°C to 520°C. This procedure eliminates surface roughness and damage induced by RIE, but, most importantly, modifies the morphology and improves the homogeneity of the pattern. Subsequently, 0 (reference for the effect of the Si buffer alone), 2.6, 4, and 5 monolayers (ML) of Ge were deposited at 620°C and at a fixed

rate of 0.03 Å/s on samples A, B, C, and D, respectively. An additional series of samples (E, F, G) was grown to investigate the stability of the observed features. Under otherwise identical conditions, 5 ML of Ge were deposited at 670 and 570°C on samples E and F, respectively, and 9 ML at 570°C on sample G. The denoted substrate temperatures were calibrated with a thermocouple embedded into a Si reference wafer to an estimated accuracy of ±15°C. Since the rate for Ge deposition is at the lower limit of our flux controller, we further enhanced the migration of the deposited Ge atoms or dimers by growth interruption for 10 s after each deposited ML. Afterwards, the substrate temperature was quickly decreased, and the surface morphology was characterized *ex-situ* with a Digital Instruments atomic force microscope (AFM) in the tapping mode.

Results

Sample	A	B	C	D
Ge Coverage (ML)	0	2.6	4	5
Morphology	Faceted Inverted Pyramid	Corrugations Without Pyramid[1]	Corrugations With Pyramid[2]	Corrugations With Dome[3]

Tab. 1: Shows the morphological evolution in the samples with different Ge coverage.

[1]As exhibited in the AFM images in Fig. 1(a) and (b);
[2]As exhibited in the 3D model in Fig. 2;
[3]As exhibited in the AFM images Fig. 1(c) and (d);

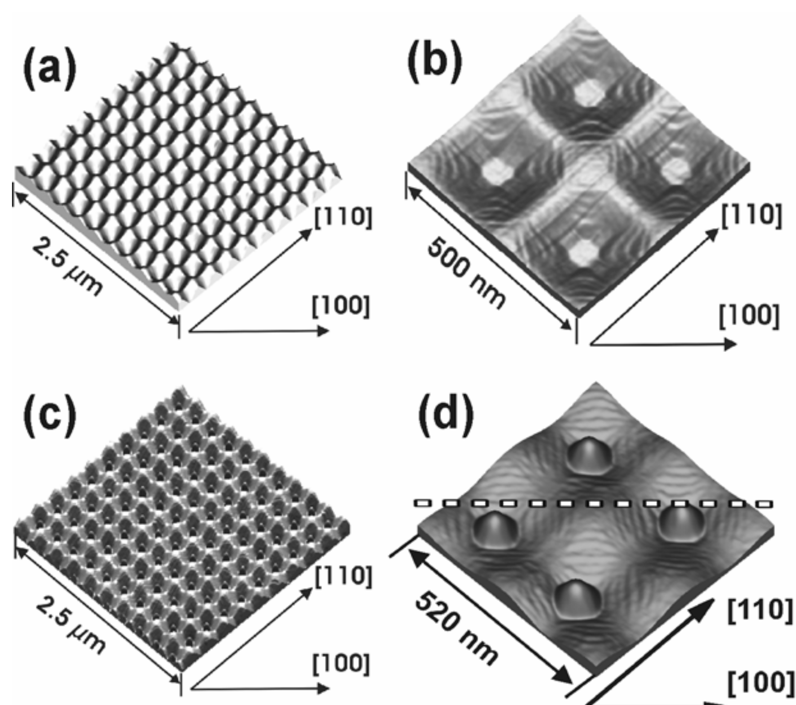

Fig. 1: AFM images in different scale for the pits after 2.6 ML Ge deposition [(a) and (b)]; after 5 ML Ge deposition [(c) and (d)], respectively..

The experiments showed that the initially forming Ge wetting layer develops a complex, but highly symmetric morphology on the inclined sidewalls of the pits [as described in Table 1].

This pattern is driven by strain- and surface energy minimization, and leads after the deposition of typically three monolayers of Ge to a conversion of the pit sidewalls into a pattern that consists exclusively of {105} and (001) facets. We attribute the subsequent islands nucleation to Ge accumulation at the bottom of the pits, which is driven by capillarity and the enhanced surface diffusion on the by now {105} faceted sidewalls of the pits. This complex interplay of mechanism in the confined geometry of the pits leads to preferential dot nucleation at the bottom of the pits despite the disadvantages of this site in terms of strain relaxation.

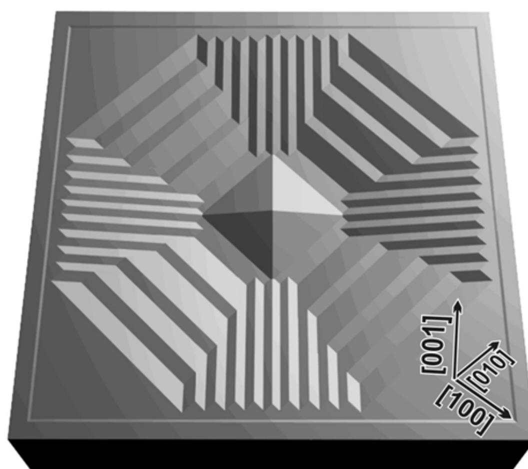

Fig. 2: Schematic 3D representation of the pit structure after the surface is converted into {105} and (001) facets. The central pyramid is pointing outwards. The 3D effect is seen best in the upper right corner.

Conclusion

The results show that SK growth in combination with nanostructured surfaces can be exploited for the implementation of perfectly ordered SiGe and Ge nanostructures that fulfill basic preconditions for meaningful device applications, namely addressability.

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