Evolution of shape, height and in-plane lattice constant of Ge-rich islands during capping with Si


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The morphology of Ge-rich islands on Si (001) substrates capped with 0 to 10 monolayers (MLs) of Si at 550°C was investigated. An evolution of the island shape from domes to pyramids observed by atomic force microscopy (AFM) coincides with a dramatic decrease of the island height during overgrowth. As an explanation for the mechanism, Si incorporation into Ge islands during the initial growth of Si cap layer was suggested [1,2], but so far has not been directly verified. Therefore we measured the average lateral lattice constant $\langle a_{||} \rangle$ of the islands from grazing incidence x-ray diffraction (GID) at an x-ray wavelength of 1.5496 Å at the beamline BW2.

The reference sample without Si cap exhibits dome-shaped islands with very uniform size. With a 1.3 ML thick Si cap layer, the base of the islands becomes pyramid-like shape, while the upper part remains dome-like. Further Si deposition leads to a change of the island shape to a pyramid, and finally, for the thickest cap layer of 10 ML’s of Si, the shape of the islands is transformed to ‘T pyramids’. These observations correspond well to a scanning tunnelling microscopy study by Rastelli et al. [1,3].

Figure 1(a) shows the height histograms of the islands for all. No apparent bimodal size distribution is observed, indicating that the shape transformation during capping occurs very quickly. The average height of the islands versus cap thickness is shown in Fig. 1(b). The height of the islands significantly decreases with Si overgrowth. As a first approximation, we assume that the deposited Si atoms on the Ge islands prefer to migrate away toward the wetting layer (WL) between the islands. In the extreme case, if all Si atoms deposited in the area occupied by Ge islands migrate to the WL, the WL thickness will increase, and the height of the islands above the WL would accordingly decrease as depicted by the open circles in Fig. 1(b).

![Figure 1](image-url)

Figure 1: (a) island height distribution measured by AFM. (b) decrease of the average island height with Si cap thickness (solid squares) compared to a simple simulation (open circles, see text).

Obviously, the experimentally determined heights are remarkably smaller than the estimated value, especially for 2.4, 6, and 10 ML Si cap layer. Therefore, the height decrease can only be explained by a mass transport from the island apex to their sides and to the area between the islands, i.e., by Ge transport from the apex of the islands, as well as a partial transfer of the deposited Si. This mass transport does not occur in a continuous manner. We rather observe a sharp drop in island height for capping with 2.4 ML Si. Just at this stage, the island shape changes from dome to pyramid. Therefore, we obtain the following picture for island capping: in the first stage, material is effectively attached at the island boundaries. Mass transport from the island apex to the base boundary occurs at a relatively slow rate. After a certain amount of Si incorporation, this mass transport occurs considerably faster, indicating Ge migration from the island apex to the sides of
the islands and to the regions between the islands. In other words, the deposited Si atoms seem to act as a “catalyst”, stimulating the detachment of Ge atoms from the island apex. In Refs. 1 and 3, this process was attributed to a “phase transition” between different equilibrium island shapes at different strain values (due to an increasing amount of Si in the islands).

For a direct evidence for intermixing, we measure the average lateral lattice constant \( \langle a \rangle \) of the islands using GID, as shown in Fig. 2. Two truncation rods (TR) are observed, one at about \( Q_x = 4.628 \) Å\(^{-1} \), corresponding to the Si substrate and the wetting layer, and one at about \( Q_x = 4.57 \) Å\(^{-1} \), related to the islands. To observe the exact TR position of the islands, reciprocal space maps in the \( Q_x-Q_y \) plane at \( Q_z = 0.0155 \) Å\(^{-1} \), [indicated by a black line in Fig. 2(a)] are shown in Fig. 2(b-f).

From the intensity maxima in these maps, we obtain \( \langle a \rangle \) of the islands as a function of the cap layer thickness, shown in Fig. 2(g).

![Figure 2](image)

Figure 2: (a) \( Q_x-Q_z \) reciprocal space map of the reference sample in GID geometry. Two truncation rods from the substrate and the island are visible. (b)-(f) in-plane \( Q_x-Q_y \) reciprocal space maps for the sample series: the island peak shifts toward the substrate peak with increasing Si cap thickness. (g) average in-plane lattice parameter \( \langle a \rangle \) of the islands as a function of cap layer thickness.

Apparently, \( \langle a \rangle \) decreases during Si overgrowth. As \( \langle a \rangle \) depends on both, the island composition as well as the island strain state, we cannot directly conclude on the composition. However, simulations of island relaxation based on the finite element method showed that for a given composition the strain in the islands depends mainly on their aspect ratio: the higher the aspect ratio \( h/r \), the better the islands can elastically relax, and hence the larger is the in-plane strain with respect to the substrate \( \varepsilon|| = \langle a \rangle - a_{Si} / a_{Si} \). While the island shape and aspect ratio are almost unchanged for 1.3 ML Si cap as compared to the uncapped sample, \( \langle a \rangle \) decreases already significantly. This decrease can therefore only be an effect of reduced Ge content in the islands, thus suggesting Si incorporation into the islands. The coincidence of the rather abrupt shape change at about 2 ML coverage with the considerable Si interdiffusion is a clear experimental support of the reasoning given in Ref. 1 that intermixing drives the transition of island shape from dome to pyramid during Si capping. For coverages above 2.4 ML, both the aspect ratio as well as \( \langle a \rangle \) decrease at a moderate rate, and we cannot quantitatively conclude on composition changes.

References