Island formation during lattice mismatched heteroepitaxy: Experimental observations
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Kinetic Pathway in Stranski-Krastanov Growth of Ge on Si(001)
Y.-W. Mo, D. E. Savage, B. S. Swartzentruber, and M. G. Lagally
University of Wisconsin–Madison, Madison, Wisconsin 53706
(Received 21 April 1990)

The transition from 2D to 3D growth of Ge on Si(001) has been investigated with scanning tunneling microscopy. A metastable 3D cluster phase with well-defined structure and shape is found. The clusters have a [110] facet structure. Results suggest that these clusters define the kinetic path for formation of “macroscopic” Ge islands.

475° C, > 3 ML Ge

FIG. 2. STM images of single “hut” cluster. (a) Perspective plot. Scan area is 400 Å × 400 Å. The height of the hut is 28 Å. (b) Curvature-mode grey-scale plot. The crystal structure on all four facets as well as the dimer rows in the 2D Ge layer around the cluster are visible. The 2D layer dimer rows are 45° to the axis of the cluster.
**Dislocation-Free Stranski-Krastanow Growth of Ge on Si(100)**

D. J. Eaglesham and M. Cerallo  
AT&T Bell Laboratories, 600 Mountain Avenue, Murray Hill, New Jersey 07974  
(Received 27 December 1989)

We show that the islands formed in Stranski-Krastanow (SK) growth of Ge on Si(100) are initially *dislocation-free*. Island formation in true SK growth should be driven by strain relaxation in large, dislocated islands. Coherent SK growth is explained in terms of elastic deformation around the islands, which partially accommodates mismatch. The limiting critical thickness, \( \tilde{h} \), of coherent SK islands is shown to be higher than that for 2D growth. We demonstrate growth of dislocation-free Ge islands on Si to a thickness of \( \approx 500 \) Å, 50\% higher than \( \tilde{h} \), for 2D Ge/Si epitaxy.

![Image 1: Schematic diagram of the three possible growth modes: Frank-van der Merwe, Volmer-Weber, and Stranski-Krastanow. Where interface energy alone is sufficient to cause island formation, VW growth will occur. SK growth is uniquely confined to systems where the island strain energy is lowered by misfit dislocations underneath the islands.](image1.png)

![Image 4: Plan-view and cross-section TEM images of large coherent SK islands close to their maximum size prior to dislocation introduction. (a) Bright-field image near the (100) Bragg position showing characteristic “beard-collars” contrast due to dome-shaped deformation of the substrate around the island. (b) (400) dark-field image; note strong strained contrast around island.](image4.png)

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**Self-assembled quantum dots**

- **Deposition in Ultra-High-Vacuum (UHV)**
- **Stranski Krastanow growth**
  - Smaller lattice constant, larger band gap: e.g., Ge, InAs, InP
  - Larger lattice constant, smaller band gap: e.g., Si, GaAs, GaInP

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**Perfect crystallinity of islands**
Typical quantum dot distribution

6 ML Ge on Si (001) at 700 °C

2 x 2 µm²

The pyramid precursor

<table>
<thead>
<tr>
<th>Prepyramid</th>
<th>Transition shapes</th>
<th>Truncated pyramid</th>
</tr>
</thead>
<tbody>
<tr>
<td>115×115×1.7 nm³</td>
<td>70×70×2.5 nm³</td>
<td>90×90×3.3 nm³</td>
</tr>
<tr>
<td>90×90×4.3 nm³</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

In the high temperature regime, islands form as unfaceted prepyramids and then transform into truncated {105} faceted pyramids with a rough top (T pyramids).

The transition from pyramid to dome

<table>
<thead>
<tr>
<th>Pyramid</th>
<th>Transition shapes</th>
<th>Dome</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Pyramid" /></td>
<td><img src="image2" alt="Transition shapes" /></td>
<td><img src="image3" alt="Dome" /></td>
</tr>
<tr>
<td>{105}</td>
<td>{113}</td>
<td>{15 3 25}</td>
</tr>
<tr>
<td>Atoms diffuse towards apex (ab-initio). Step-flow growth of {105} facets</td>
<td>At a critical size {105} facets are not completed any more.</td>
<td>Step bunching on {105} facets. Formation of new, steeper facets.</td>
</tr>
<tr>
<td>Fully developed multi-faceted dome.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>


The transition from dome to barn

![Diagram](image4)

Stability of island ensemble

6 ML Ge @ 850°C
(large material transport on surface)

Trenches allow shrinking islands to be identified: footprints of the island evolution!

Non-similar island shrinking

Shrinking islands: P — TP — PP

Reversible process compared to growing islands!

Natural result in a thermodynamic picture.


Where does material of shrinking islands go?

Material preferably goes to nearest neighbours.
Trench formation around SiGe islands


Dendrochronology of Strain-Relaxed Islands

(Study of tree rings)

Max Planck Institut für Festkörperphysik, Heisenbergstrasse 1, D-70569 Stuttgart, Germany
(Received 10 December 2005; published 6 June 2006)

Douglas-fir (photo H.D. Grissino-Mayer)

Probing the lateral composition profile of SiGe islands

Before etching
After selective etching
(2 min in 31% H₂O₂)

Grown at 560 °C

6 ML Ge at 560 °C, 500 s GI

Trenches after post-growth annealing (in-situ)

10 ML Ge at 740°C

After 2 min. etching in HF/H₂O₂/CH₃COOH (BPA solution)
+ 1 min. anneal 740°C
+ 10 min. anneal 740°C

- Before annealing: Si plateau at the center of the trench
- After annealing: only a part of the initial Si plateau remains and a wide shallow trench appears

Island motion

Lateral SiGe island motion during in-situ annealing


Cross-section AFM

Evidence of asymmetric alloying
Wet chemical etching in a NH₄OH/H₂O₂ solution (selective etching of SiGe alloys)

- Ge rich part at the left side of the island
- Si rich part at the right side of the island

Island motion: efficient Si-Ge intermixing by surface diffusion
Lateral SiGe island motion during in-situ annealing

Mean island displacement

- Short annealing times: rapid island motion
- Island motion slows down for annealing times > 20 min.

Once the island has intermixed, lateral motion ceases

Probing the lateral composition profile of SiGe islands

Before etching

After selective etching
(2 min in 31% H$_2$O$_2$)

Grown at 560 °C

6 ML Ge at 560 °C, 500 s GI

Does motion depend on environment?

10 ML Ge + 1 min annealing @ 740°C (+2 min BPA)

Neighboring islands “repel” each other

All islands
Nearest neighbour at distance D < 250 nm

Can we suppress island motion?

- Island motion suppressed for thin spacer layers
- For thicker spacer layers: Island motion gradually recovers to values measured for single layers

The “etching solution”

Selective etching - NH$_4$OH:H$_2$O$_2$

Rates measured on relaxed SiGe buffers, but islands are strained!

Etching rate for biaxially strained (20%) SiGe films – Insensitivity of etching rate to strain

$R_{(c)} = \Delta h(x,y,z) / \Delta t = c(x,y,z)$

Calibration of $R_{(c)}$


Etching sequence

15 ML Ge at 740 °C

Etching time: 0, 6, ..., 270, 290 min

AFM images of the same area are background corrected and overlapped using center of trenches as control points

Local etching rate?

AFM Scale: 1670 x 2150 x 107 nm$^3$
Horizontal Slices of 3D islands

Nano Letters 8, 1404 (2008)
Vertical Cuts

Coherent islands: Ge rich top + asymmetry (sample dependent)
Superdomes: Ge rich core and alloyed periphery

Local Ge fraction $x$

0.1 0.42

Revealing the details of capped SiGe islands

5.9 ML Ge, 580 °C

20 nm Si 2x2 μm²

2x2 μm² 450°C

After Si cap etching

Composition profile

Although islands look completely different after capping, they remain practically unchanged below the Si !!!

G. Katsaros et al.,
APL 89, 253105 (2006)
**Bimodal island distribution**

6 ML Ge on Si (001) at 700 °C

Growth rate: 0.01 ML/s


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**InAs QDs: Bimodal island distribution**

2 ML InAs on GaAs (001) at 500 °C

Growth rate: 0.01 ML/s
Close look at island formation in both material systems

Ge / Si(001)  
InAs / GaAs(001)

Domes

\{105\}  
\{113\}  
\{15 3 23\}

Domes

\{137\}  
\{101\}  
\{111\}

Universal island shapes in two model material systems

Ge / Si(001)  
InAs / GaAs(001)

Pyramid  
Dome

\{105\}  
\{113\}  
\{15 3 23\}  

Pyramid  
Dome

\{137\}  
\{101\}  
\{111\}

- Small faceted islands are pyramids with 4 shallow \{105\} ((137)) facets.
- At a critical size, pyramids transform into multifaceted steeper islands (domes) through intermediate shapes.
- Domes have \{113\} and \{15 3 23\} (or \{111\} and \{101\}) at their body and small \{105\} ((137)) at foot and top (as predicted by I. Daruka, J. Tersoff, PRB 66 (2002) 132104.)

Alloyed island growth (pyramids)

Si$_{0.5}$Ge$_{0.5}$  In$_{0.5}$Ga$_{0.5}$As

Ge/Si (InAs/GaAs) islands overgrowth with Si (GaAs)

A.Rastelli et al, PRL 87 (2001) 256101
Ge/Si islands on patterned Si (001)

Pattern + buffer + 5 ML Ge + 8 ML Ge

1200 x 1200 nm²

Secondary island formation


Thank you!