Kinetic Monte Carlo Simulation of GaAs Homoepitaxy and Droplet Epitaxy

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Motivation: Ga Droplet Epitaxy

- Model liquid droplet epitaxy

Substrate Growth:

Droplet Formation:

Recrystallization:

The Model and Simulation

- Bond-counting kinetic Monte Carlo formulation
- On 2D analog of a Zincblende lattice
- **Atomistic, explicit two species (Ga and As) simulation**
Simulation Results: $T = 581^\circ C$

As/Ga Flux Ratio

$R_{As}/R_{Ga} = 4$

$R_{As}/R_{Ga} = 3$

$R_{As}/R_{Ga} = 2$

$R_{As}/R_{Ga} = 1$
Homoepitaxial Growth: As vs. Ga terminated surfaces

Calibrate the model to what’s observed in experiments:

- Stepflow growth
- Surface reconstruction, or 2D analog of this.

*Courtesy: L. Däweritz and R. Hey*
Homoepitaxial Growth: As vs. Ga terminated surfaces

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As vs. Ga terminated surfaces: Simulation

- Simulated 10 seconds of growth with fixed flux $R_{Ga} = 0.58$ monolayers/second.
- Sampled last 3 seconds at periodic intervals and calculated percent surface Ga.
- Varied As flux $R_{As}$ and temperature $T$:

$$\frac{R_{As}}{R_{Ga}} \in [1, 10],$$
$$T \in [436, 627]^\circ C.$$
Simulation Results: Phase Diagram

\[ R_{\text{As}} / R_{\text{Ga}} \]

\[ T^{-1} (K^{-1}) \times 10^{-3} \]

\[ 10^0 \quad 10^1 \]

Introduction

GaAs Homoepitaxial Growth

Future Work
Simulation Results: Phase Diagram

\[ \frac{R_{\text{As}}}{R_{\text{Ga}}} \]

\[ T^{-1} \quad (\text{K}^{-1}) \times 10^{-3} \]
Droplet Epitaxy

- Various phenomena associated to droplet epitaxy (e.g. Etching, Rings)
- Simulate droplet crystallization

Ring Formation in Experiments:

**FIG. 1.** (Color online) (a) AFM image of the 3.5 ML Ga droplets. AFM images of GaAs nanorings formed at (b) 150 °C, (c) 200 °C, and (d) 350 °C, respectively.

Droplet Epitaxy