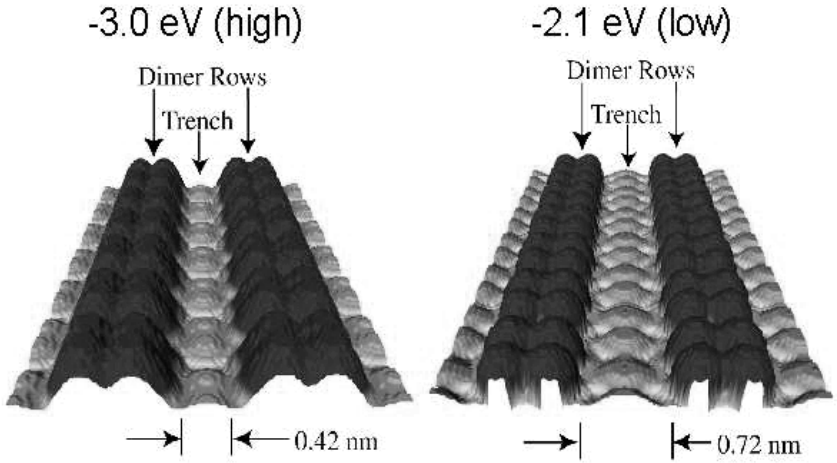
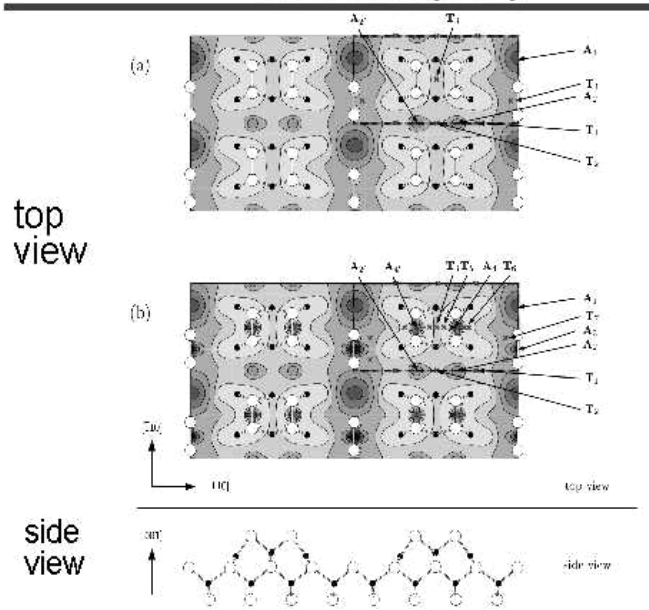
Voltage dependence of the STM current

STM simulation



*LaBella, Yang, Bullock, Thibado, Kratzer & Scheffler, PRL **83**, 2989 (1999).*

Total energy of a diffusing Ga atom at GaAs (001)



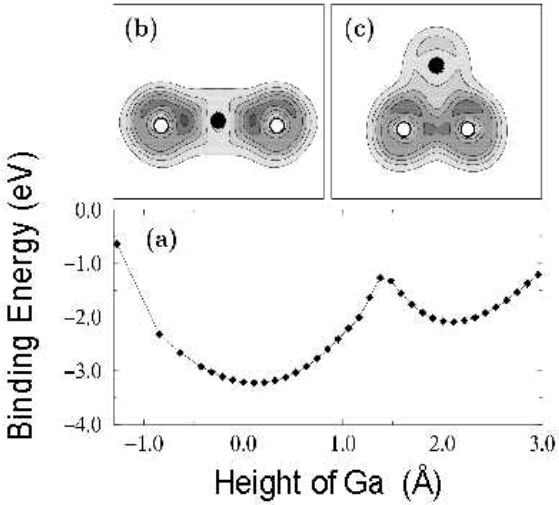
E_{A1} = -2.5 eV
E^{TS} = -2.0 eV

E_{A2} = -2.2 eV
E^{TS} = -1.8 eV

E_{A3} = -3.2 eV

A. Kley, P. Ruggerone, and M.S., PRL **79** (1997)

Unusally stable site for Ga adatom inside the trench-site As-dimer

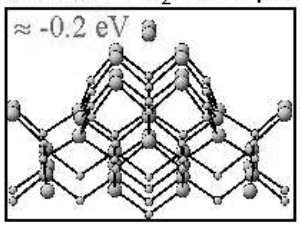


*A. Kley, P. Ruggerone, M.S., PRL **79** (1997)*

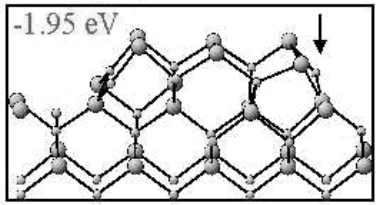
As_2 Adsorption

C. Morgan, P. Kratzer, M.S., PRL **82** (1999)

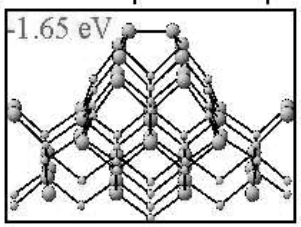
molecular As_2 adsorption



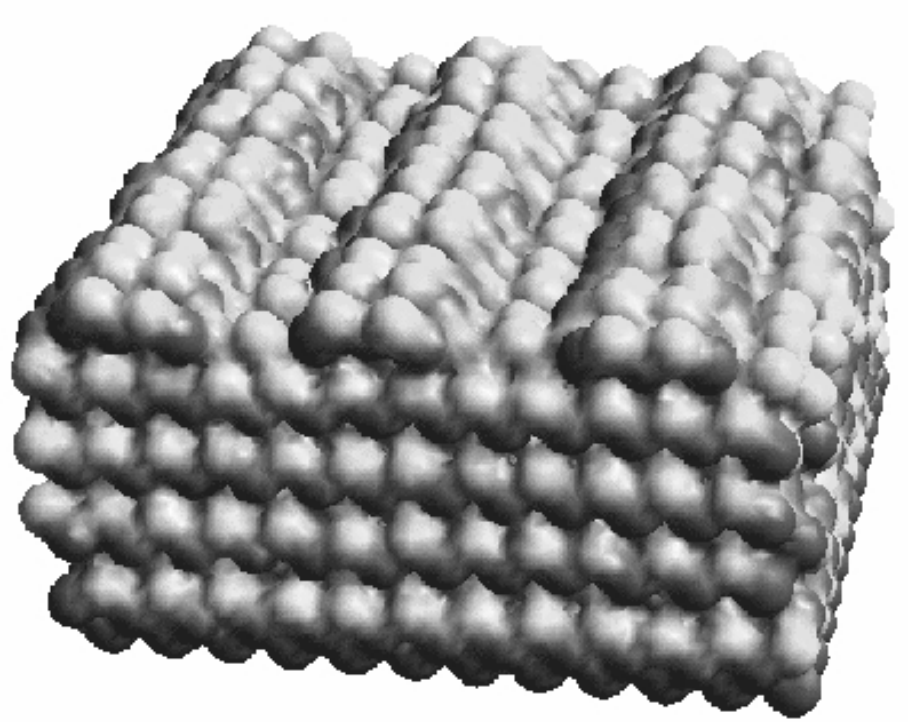
As_2 chemisorption at Ga adatom



As_2 chemisorption in top layer



As_2 does not need to break up to become incorporated. As_2 is readily available everywhere on the surface



Theory of the kinetics of growth

1) Analysis of all possibly relevant processes
2) Calculate the rates of all important processes

$$\Gamma^{(i)} = \Gamma_0^{(i)} \exp\left(\Delta E^{(i)} / kT\right)$$

3) Statistical approach to describe
   - deposition
   - diffusion
   - nucleation
   - growth

➡ **kinetic Monte Carlo method**

Summary

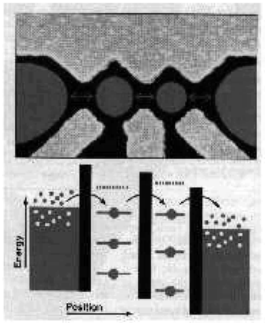
What makes GaAs(001) the preferred substrate?

- principal structural element: As dimers
  - As_2 molecules are incorporated undissociatedly and without an activation barrier
  - several intermediate binding sites enhance the As_2 surface lifetime
- unusually stable two-fold coordinated cation adsorption state
  - cation evaporation is negligible even at high growth temperatures

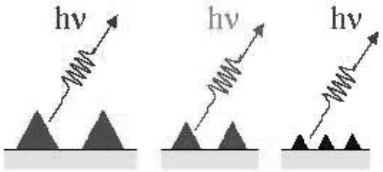
Self-Assembly of Nano-Scale Structures at Semiconductor Surfaces

Motivation:

Single-electron transistor

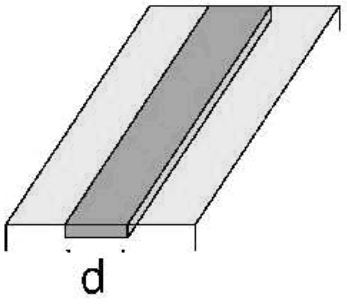


LEDs and laser diodes



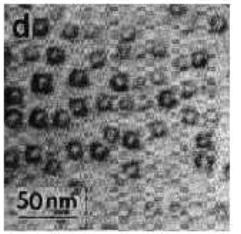
required dimensions: 50 - 200 Å

lithography ends at d > 300 Å, and has rough edges



self-assembly of InAs quantum-dots on GaAs (100)

Ruvimov et al., PRB 1995

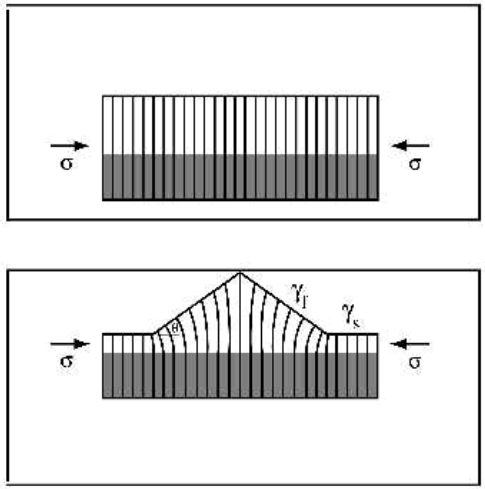


Thermal Equilibrium Shapes of InAs Quantum Dots on GaAs(100)

Stranski-Krastanov Growth Mode

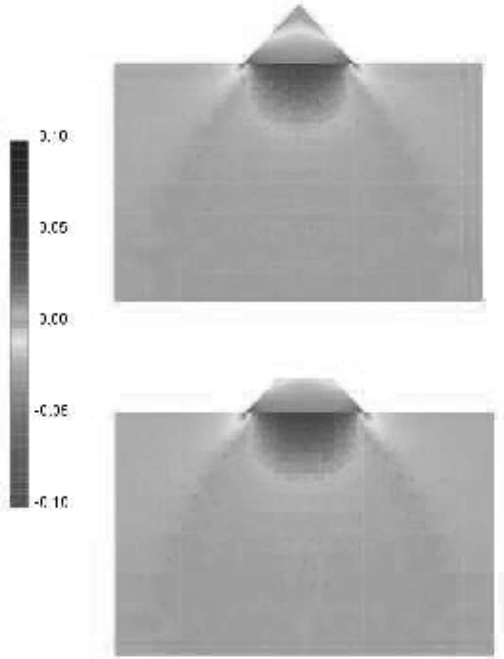
If the experimental quantum dot shape deviates from the equilibrium shape, equilibrium thermodynamics is not adequate to describe the island formation and size distribution

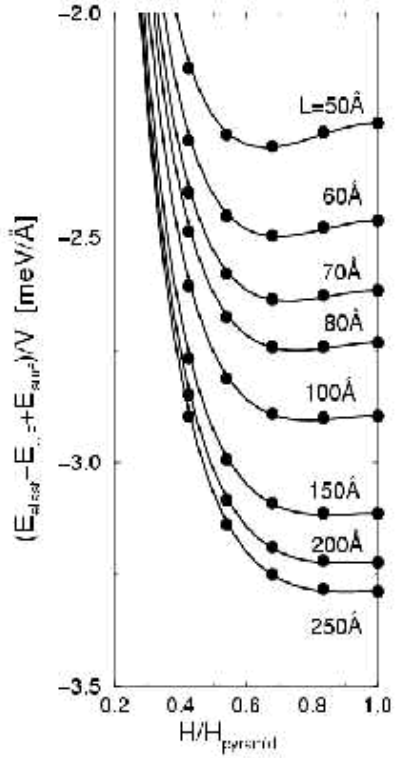
Stranski-Krastanov morphology
as one way to reduce misfit strain energy



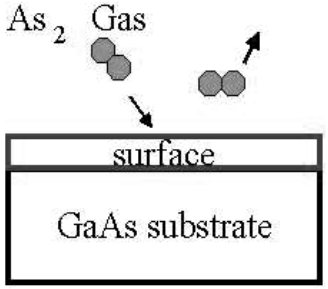
e.g.
InAs on
GaAs

Stress tensor at strained InAs on GaAs



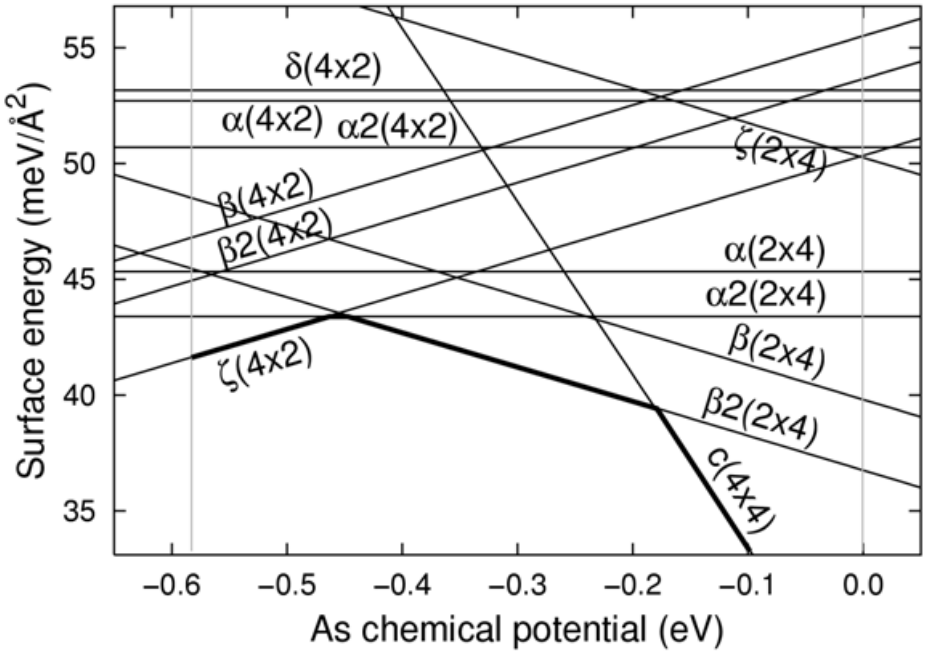


Stoichiometry and structure of the surface depend on the environment
(atomic chemical potentials)



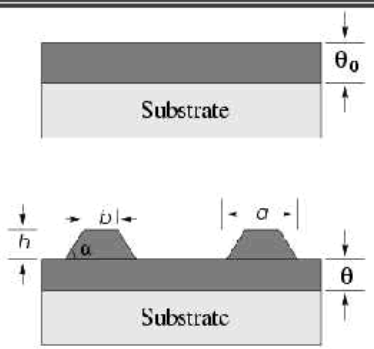
$$\mu_{\mathrm{As}} < E^{\mathrm{bulk}}(\mathrm{As})$$
$$\mu_{\mathrm{Ga}} < E^{\mathrm{bulk}}(\mathrm{Ga})$$

$$\mu_{\mathrm{Ga}} + \mu_{\mathrm{As}} = E^{\mathrm{bulk}}(\mathrm{GaAs})$$



What determines the volume and shape of quantum dots? (how q-dots eat from the wetting layer)

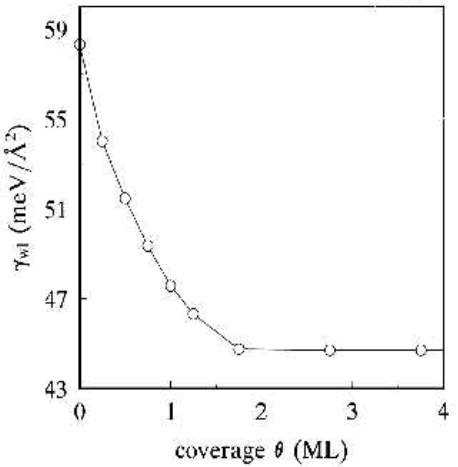
e.g. InAs on GaAs



L. Wang, P. Kratzer, and M.S., PRL 82 (1999)

$$E/V = E^{\mathrm{cl}}_{\mathrm{is}}/V - c^{\mathrm{cl}}_{\mathrm{film}} + [S\gamma_{\mathrm{f}} + b^2\gamma_{\mathrm{top}} - a^2\gamma_{\mathrm{wl}}(\theta_0)]/V + (1/n - a^2) \times [\gamma_{\mathrm{wl}}(\theta) - \gamma_{\mathrm{wl}}(\theta_0)]/V$$

InAs on GaAs (100)
surface plus interface energies

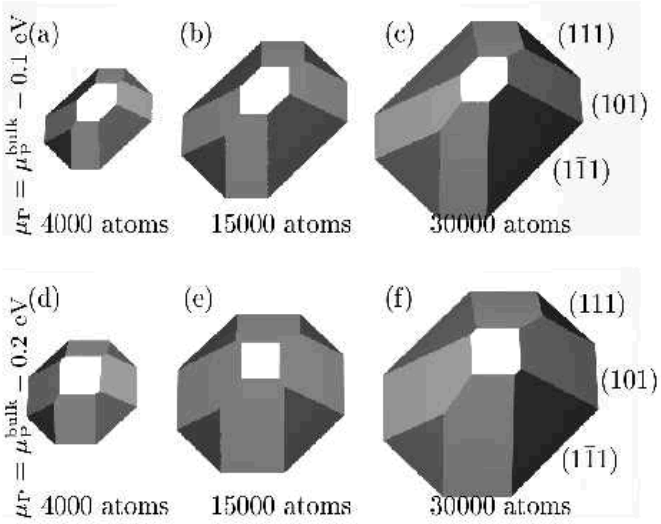


$$\gamma_{\mathrm{wl}} A = E^{\mathrm{tot}} - E^{\mathrm{bulk}}(\mathrm{GaAs})\, N_{\mathrm{Ga}} - E^{\mathrm{strained\text{-}bulk}}(\mathrm{InAs})\, N_{\mathrm{In}} - \mu_{\mathrm{As}}\, \Delta N_{\mathrm{As}}$$

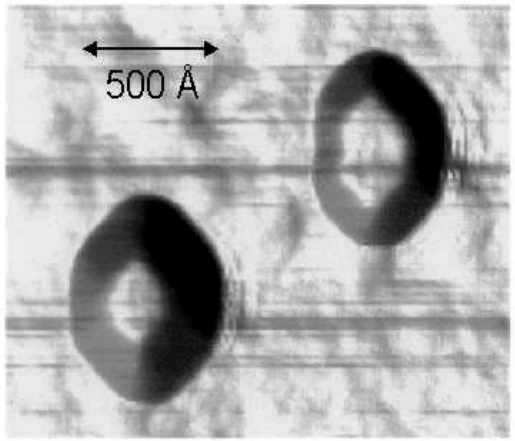
$$\mu_{\mathrm{As}} = E^{\mathrm{bulk}}(\mathrm{As}) - 0.2\ \mathrm{eV}$$

L. Wang, P. Kratzer, and M.S., PRL 82 (1999)

InP quantum dots on GaP(001)



Q. Liu, E. Pehlke, N. Moll, M.S., PRB ***60****, (1999)*



Samuelson *et al.* (1996)

MOVPE grown InP islands on GaInP

Electronic Structure Theory
(Density Functional Theory)
➡ **Potential Energy Surface**

Dynamics of the Nuclei along this **PES**

Thermal Equilibrium Structures

Statistical Mechanics

Real World