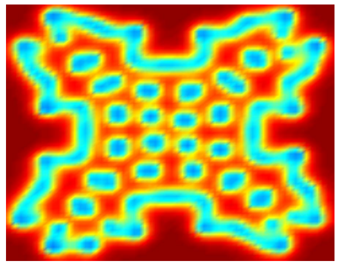
Stress Induced Patterns in Fracture, Deformation and Heteroepitaxy



From J. Pearson, "Complex Patters in a Simple System", Science, Vol. 261, pp. 189-192 (1993)

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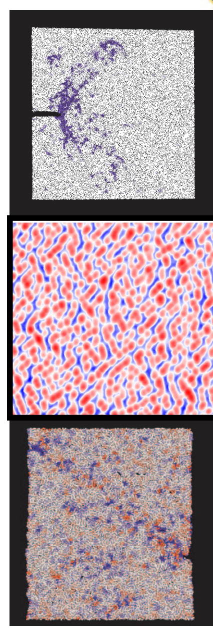
Patterns Formed Under Stress



- There are multiple examples of patterns that arise in materials systems due to the application of stress.
- The systems I will discuss include both those in which deformation leads to microstructural patterning and those in which stress coupled with diffusion drives organized nucleation.

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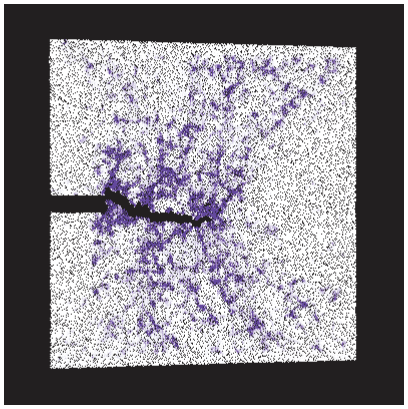
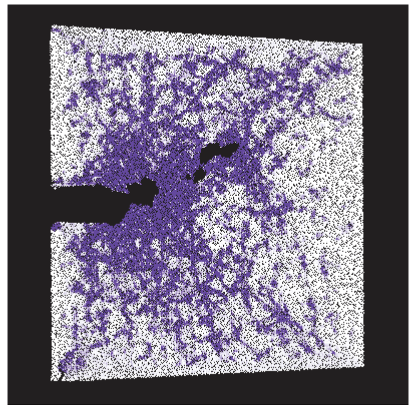
Example 1: Fracture





CLJ Potential
Brittle Fracture

Deformation:

Elastic **Plastic**

LJ Potential
Ductile Fracture

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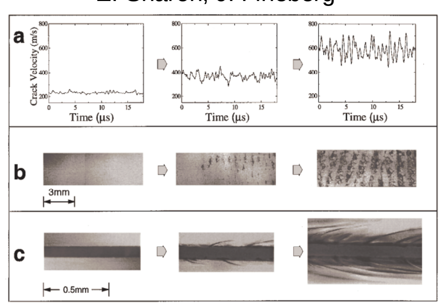
Crack Branching

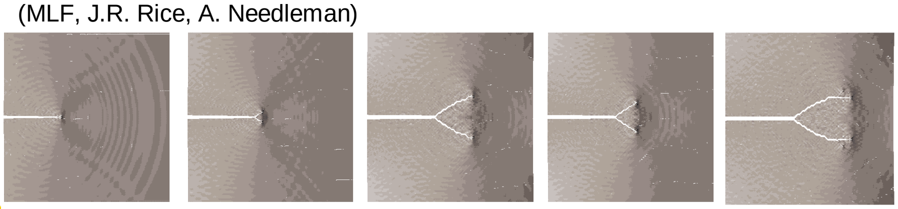
E. Sharon, J. Fineberg

Another instance in which fracture behavior defies prediction is the observed onset of branching a instability in dynamic fracture that produces daughter cracks many times larger than the inhomogeneities in the fracturing medium



V<Vc   V≳Vc   V>Vc

Cohesive Surface Simulations
(MLF, J.R. Rice, A. Needleman)



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Why are these dynamically chosen patterns so difficult to predict?

- We have two canonical theories of material behavior Hooke's Law for elastic behavior and the Navier-Stokes equation for a Newtonian fluid.
- Real solids share the qualities of both.
- Under high stresses, such as near the tips of cracks, solids flow.

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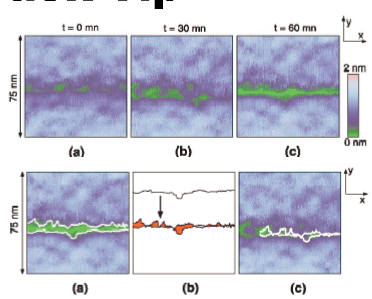
Even Silicate Glasses Flow Near The Crack Tip

To understand how a solid chooses to fracture in a brittle or ductile manner, or how a crack tip undergoes instability, we need entirely new microscopically motivated constitutive theories that capture the transfer of stability from hardening to flow.



AFM Images and Topographic Analysis showing void formation during fracture in aluminosilicate glass

from "Glass Breaks Like Metal, But at the Nanometer Scale," Celarie , Prades, Bonamy, Ferrero, Bouchaud, Guillot, and Marliere ***PRL(2003)***

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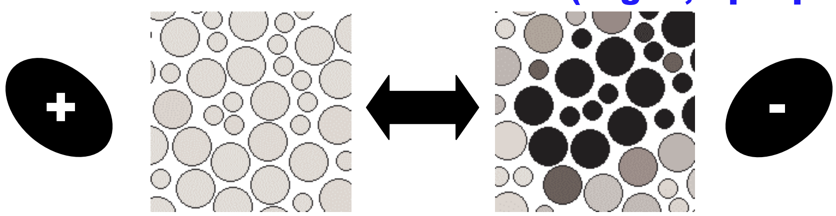
Microscopic Two-state Regions

(Argon, Spaepen)



- Region deforms locally under applied stress
- Region may reverse its rearrangement if stress is reversed shortly thereafter
- Deformation becomes permanent after some amount of additional rearrangement
- Deformation in opposite direction produces deformation in different regions

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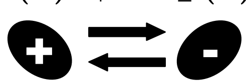
The STZ Model

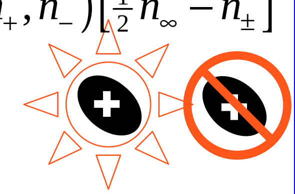
Plastic Strain Rate Proportional to Flips

$$\dot{\varepsilon}^{pl} = \Omega\left[R_-(s)n_- - R_+(s)n_+\right]$$

Master Equation for Densities

$$\dot{n}_\pm = R_\mp(s)n_\mp - R_\pm(s)n_\pm + \Gamma(s,n_+,n_-)\left[\tfrac{1}{2}n_\infty - n_\pm\right]$$





Change of Variables

$$\Lambda \equiv \frac{n_+ + n_-}{n_\infty}, \Delta \equiv \frac{n_+ - n_-}{n_\infty}$$

$$S \equiv \tfrac{1}{2}(R_- - R_+), C \equiv \tfrac{1}{2}(R_- + R_+), T = S/C$$

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The STZ Model

Plastic Strain Rate Proportional to Flips

$$\dot{\varepsilon}^{pl} = \Omega C(s)\left[\Lambda T(s) - \Delta\right]$$

Master Equation for Densities

$$\dot{\Delta} = \frac{2}{\Omega}\dot{\varepsilon}^{pl}(s,\Lambda,\Delta) - \Gamma(s,\Lambda,\Delta)\Delta,$$

$$\dot{\Lambda} = \Gamma(s,\Lambda,\Delta)(1-\Lambda).$$

Γ can be uniquely determined by resorting to basic thermodynamic arguments. (L. Pechenik)

Consequently Γ is positive definite and Λ=1 at any fixed point.

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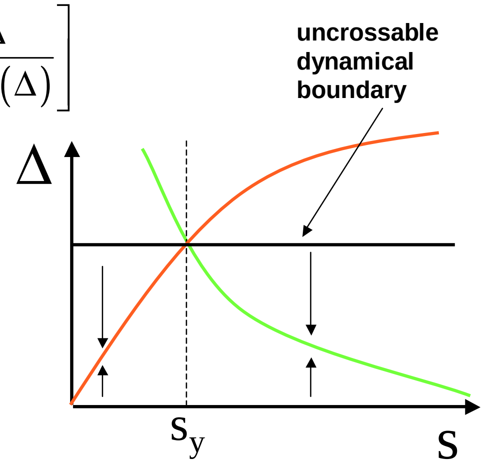
Dynamic Transition from Hardening to Flow

$$\dot{\varepsilon}^{pl} = \Omega C(s)\left[T(s) - \Delta\right]$$

$$\dot{\Delta} = \frac{2}{\Omega}\dot{\varepsilon}^{pl}(s,\Lambda,\Delta)\left[\frac{1-s\Delta}{1-\Delta T^{-1}(\Delta)}\right]$$

Jammed steady state
Δ= T(s)

Flowing steady state
Δ=1/s



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Summary: Fracture

- To understand the patterns that emerge near crack tips or under extreme deformation, constitutive equations are needed that have a real dynamical transition from hardening to flow
- The state variables of these constitutive relations should have direct foundations in microstructure.

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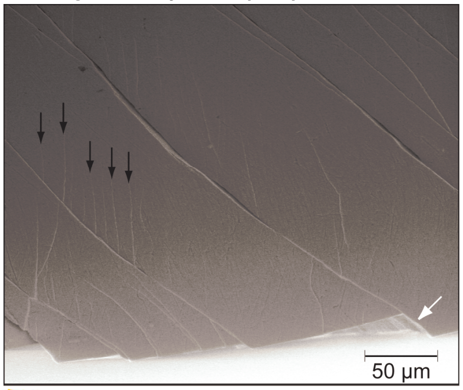
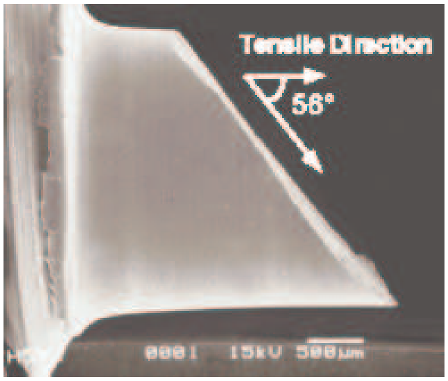
Example 2: Strain Localization

Electron Micrograph of Shear Bands Formed in Bending Metallic Glass
Hufnagel, El-Deiry, Vinci (2000)



Quasistatic Fracture Specimen
Mukai, Nieh, Kawamura, Inoue, Higashi (2002)



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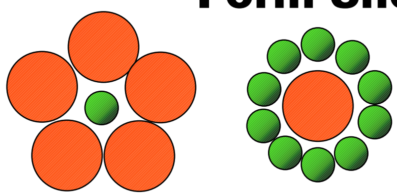
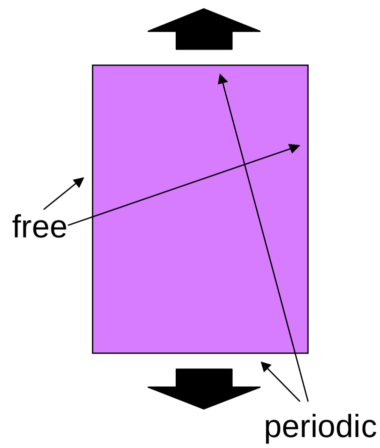
Does 2DLJ Glass Spontaneously Form Shear Bands?



- Include free boundaries in a uniaxial tensile test of our 2DLJ material.
- Experiments on metallic glass in unconstrained geometries typically exhibit shear banding. Does the 2DLJ glass?



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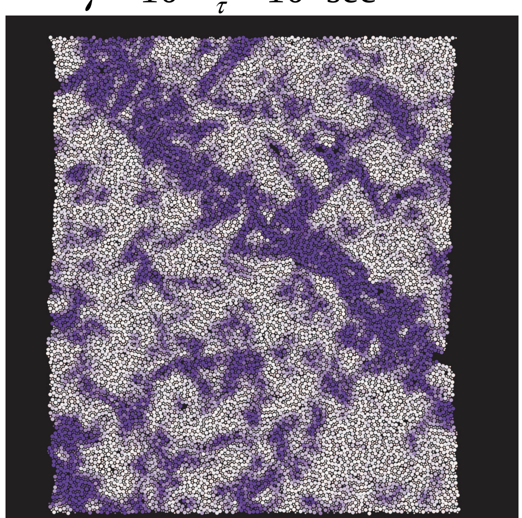
2DLJ Uniaxial Tensile Test

$$\dot{\gamma} = 10^{-5}\,\tfrac{1}{\tau} \approx 10^{7}\,\sec^{-1}$$



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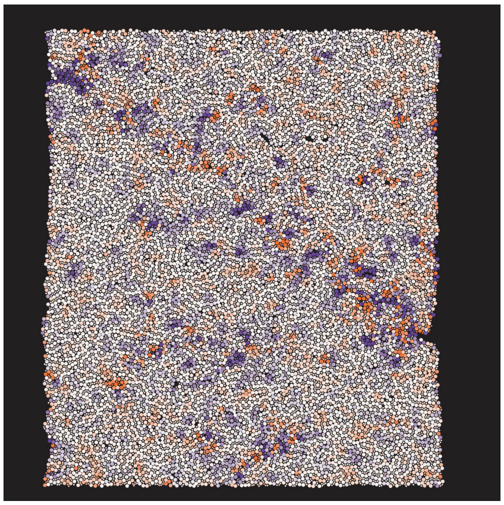
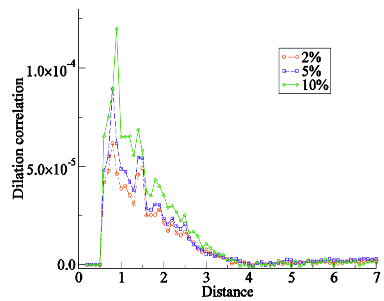
Lower Strain Rate Tensile Test
Dilation in 0.5% strain increments





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Summary: Shear Bands

- Deformation naturally couples stress and the boundary geometry leading to shape instabilities such as necking.
- The nature of the microstructural unit (the STZ) couples shear and dilation/contraction. This appears to play an important role in shear band formation.

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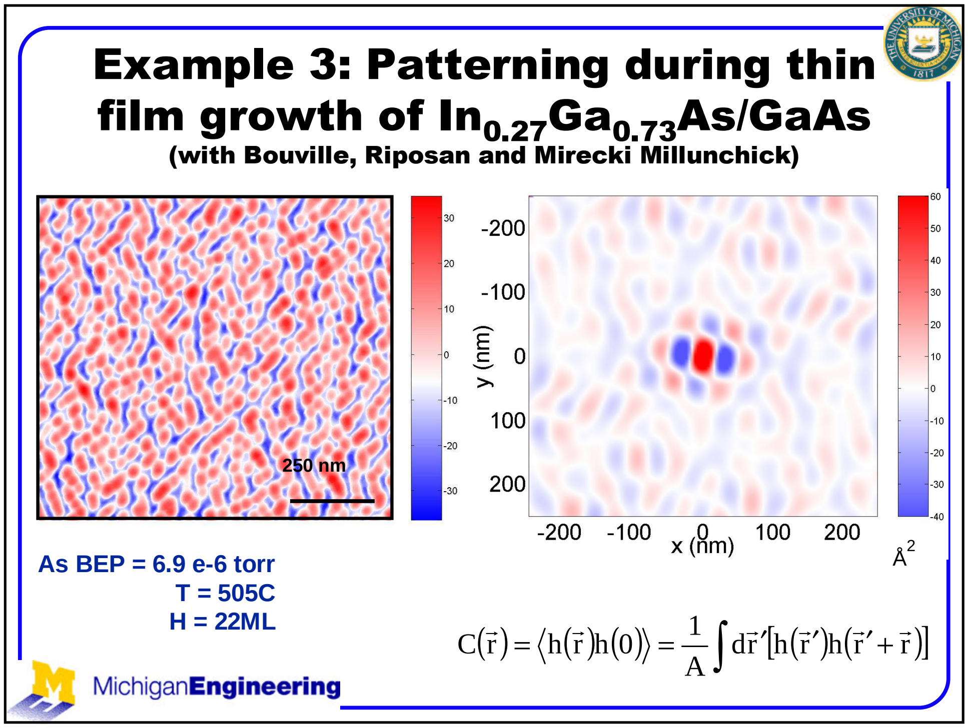
Example 3: Patterning during thin film growth of $In_{0.27}Ga_{0.73}As/GaAs$
(with Bouville, Riposan and Mirecki Millunchick)
250 nm
y (nm)
x (nm)
Å^2
As BEP = 6.9 e-6 torr
T = 505C
H = 22ML
$C(\vec{r}) = \langle h(\vec{r})h(0)\rangle = \frac{1}{A}\int d\vec{r}'[h(\vec{r}')h(\vec{r}'+\vec{r})]$
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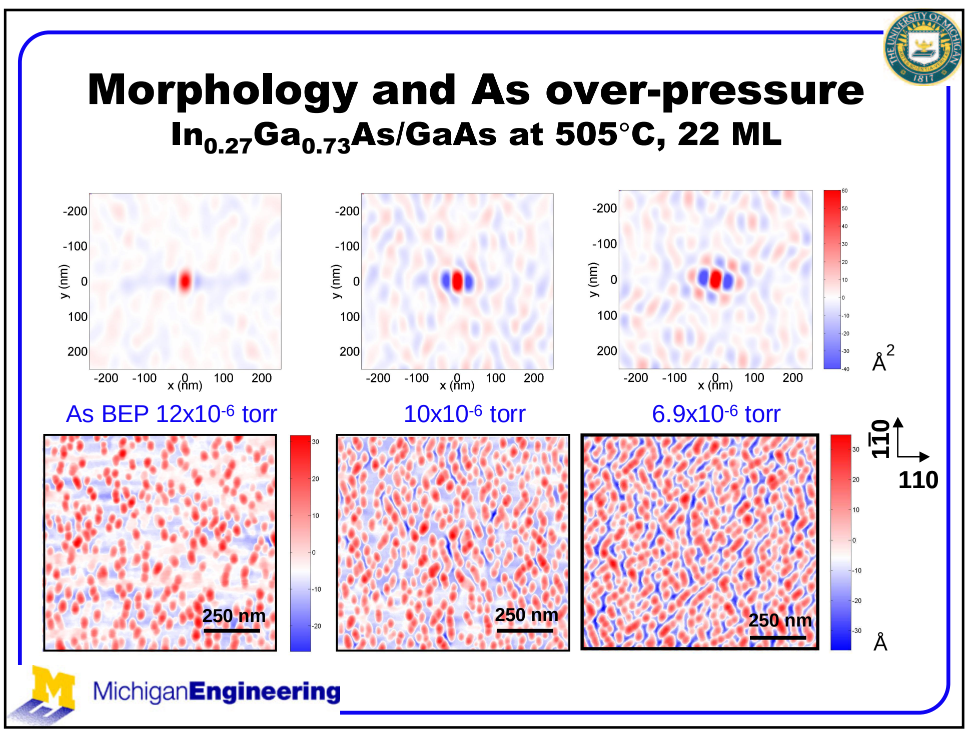
Morphology and As over-pressure
$In_{0.27}Ga_{0.73}As/GaAs$ at 505°C, 22 ML
y (nm)
x (nm)
Å^2
As BEP 12x10^{-6} torr
10x10^{-6} torr
6.9x10^{-6} torr
$1\bar{1}0$
110
250 nm
Å
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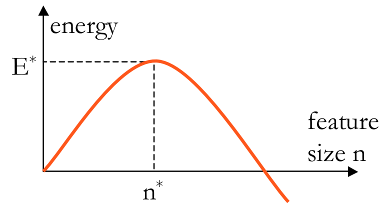
Analogy with classical nucleation theory

The energy of a cluster of size n is of the form:

$$E_n = -E_v\, n + \gamma\, n^{2/3}$$

where E_V is the volume energy and γ is the surface energy.



The critical size and the energy barrier are given by:

$$n^* = \left(\frac{2\gamma}{3E_V}\right)^3 \qquad E^* = \frac{\gamma\, n^{*2/3}}{3}$$

The energy can be rewritten as a function of n^* and E^*:

$$E_n = E^*\left[3\left(\frac{n}{n^*}\right)^{2/3} - 2\frac{n}{n^*}\right]$$

For large clusters, $\Delta E_n = E_{n+1} - E_n \approx \frac{\partial E_n}{\partial n}$

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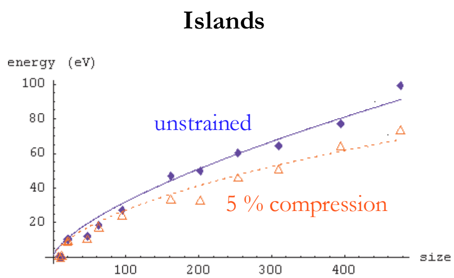
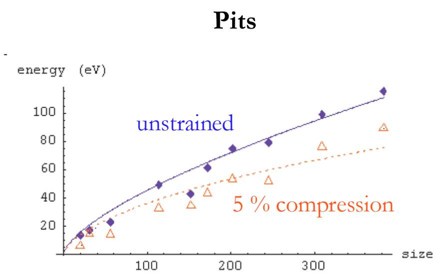
Molecular dynamics simulations: results for islands and pits





Islands:

- γ = 1.5 eV/atom
- E_v = 50 meV/atom
- $E_i^* \approx$ 210 eV
- $i^* \approx$ 8 700 atoms.

Pits:

- γ = 2.1 eV/atom
- E_v = 90 meV/atom
- $E_p^* \approx$ 160 eV
- $p^* \approx$ 3 500 atoms.

Order of magnitude ⇒ no island or pit can nucleate.

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Growth occurs in contact with a reservoir of incoming material

Islands

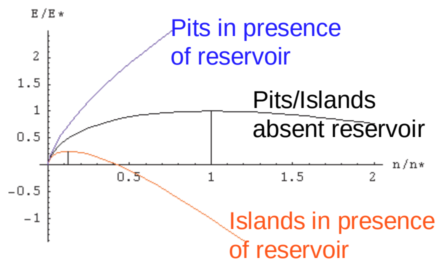
$$V_i = E_i - i\,\mu \Rightarrow i_{crit} = \frac{i^*}{\left[1+\frac{\mu}{E_V}\right]^3}$$

critical size → 1-10 atoms

Pits

$$V_p = E_p + p\,\mu \Rightarrow p_{crit} = \frac{p^*}{\left[1-\frac{\mu}{E_V}\right]^3}$$

critical size → ∞



- **Taking the chemical potential for exchange with the reservoir is important for understanding the nucleation of islands.**
- **However, this same effect seems to preclude the nucleation of pits.**

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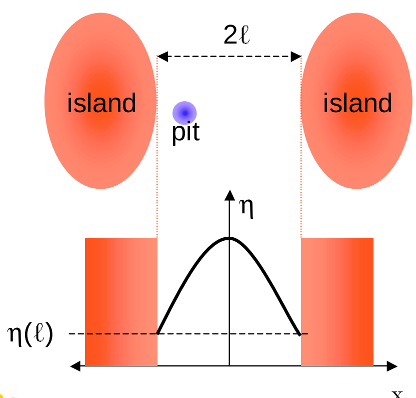
Pit nucleation takes place in the presence of islands

The presence of islands will cause inhomogeneities in the adatom concentration on the surface



- 1D diffusion equation:

$$\frac{\partial \eta}{\partial t} = D\frac{\partial^2 \eta}{\partial x^2} - \frac{\eta - \eta_e}{\tau} + F$$

  - F: flux
  - η_e: equilibrium adatom concentration $\exp(-\mu / kT)$

- Adatom concentration at a location, x:

$$\frac{\eta(x) - \eta_\infty}{\eta_{edge} - \eta_\infty} = \frac{\cosh(x/L)}{\cosh(\ell/L)}$$

  - $L = \sqrt{D\tau}$
  - $\eta_\infty = \eta_e + F\tau$

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Critical size for pit nucleation depends on the local adatom concentration

The critical pit size is determined by the net exchange in material between the pit and the surface.

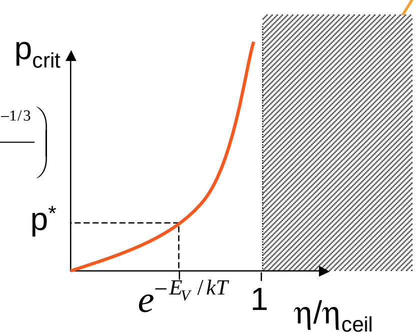
$$\frac{dp}{dt} = \nu\left(\eta_p - \eta\right)$$

$$\eta_p = \eta_e \exp\left(-\frac{\Delta E_p}{kT}\right) \approx \eta_e \exp\left(-\frac{-E_V + \frac{2\gamma}{3} p^{-1/3}}{kT}\right)$$

$$p_{crit} = \frac{-\gamma'^3}{\ln^3\left(\eta / \eta_{ceil}\right)}$$

$$\eta_{ceil} = \eta_e \exp\left(E_V / kT\right); \quad \gamma' = \frac{2\gamma}{3kT}$$

no pits will form above an adatom density, η_{ceil}



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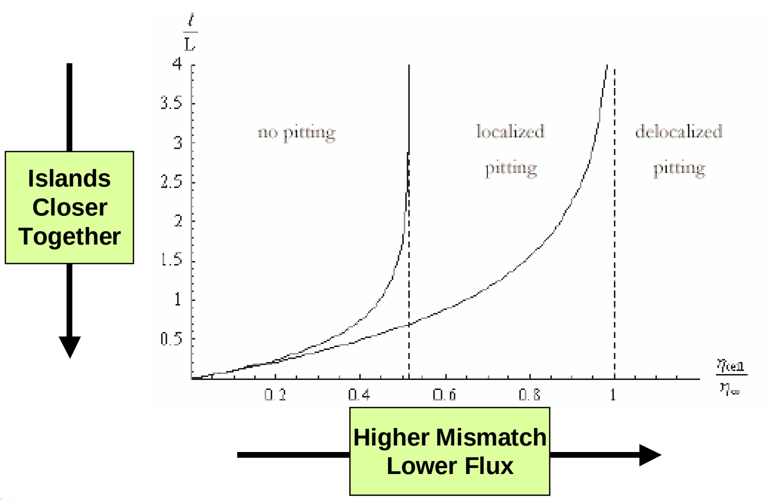
Pit Nucleation Depends on the Island-Island Separation



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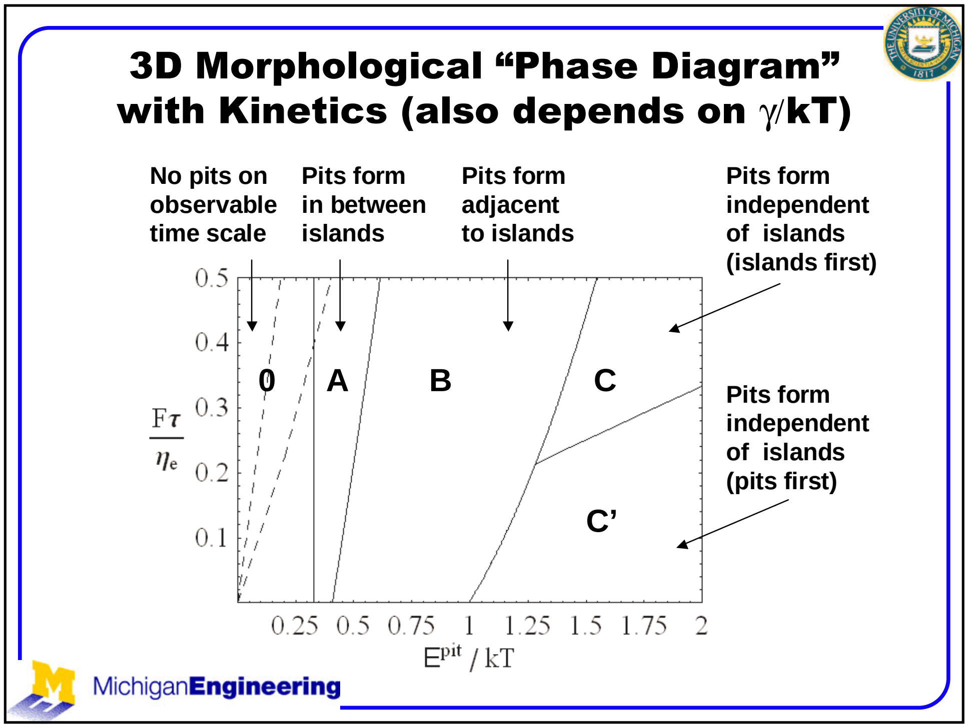
3D Morphological "Phase Diagram" with Kinetics (also depends on γ/kT)
No pits on observable time scale
Pits form in between islands
Pits form adjacent to islands
Pits form independent of islands (islands first)
Pits form independent of islands (pits first)
0
A
B
C
C'
0.5
0.4
0.3
0.2
0.1
Fτ / ηe
0.25 0.5 0.75 1 1.25 1.5 1.75 2
Epit / kT
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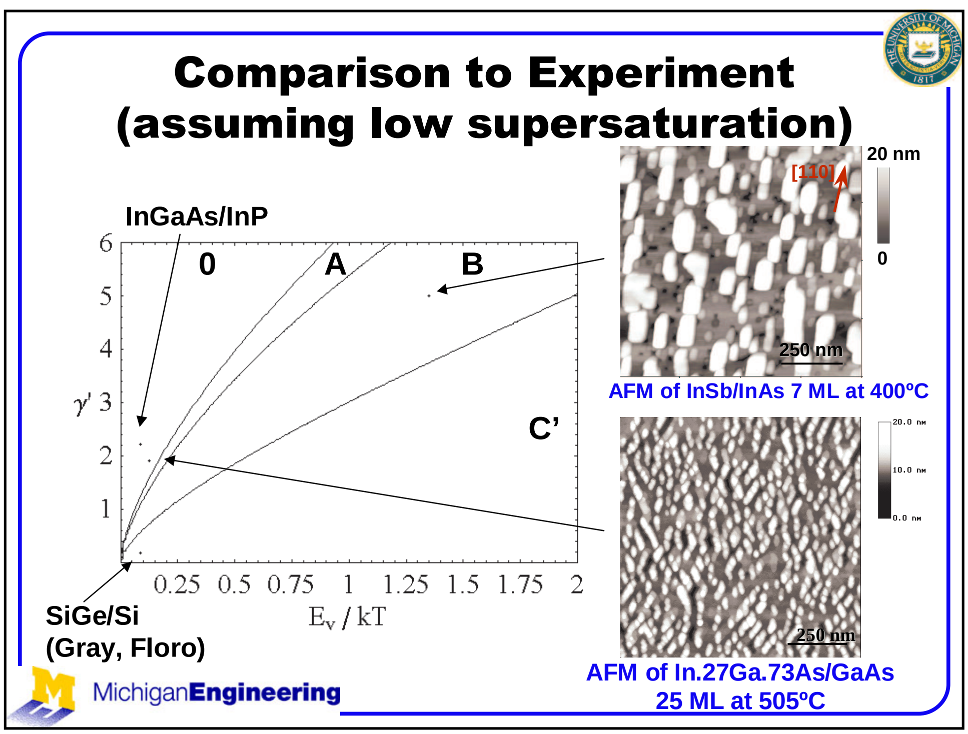
Comparison to Experiment (assuming low supersaturation)
InGaAs/InP
0
A
B
C'
6
5
4
3
2
1
γ'
0.25 0.5 0.75 1 1.25 1.5 1.75 2
Ev / kT
SiGe/Si (Gray, Floro)
[110]
20 nm
0
250 nm
AFM of InSb/InAs 7 ML at 400ºC
250 nm
AFM of In.27Ga.73As/GaAs 25 ML at 505ºC
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Summary: Pit Nucleation

- Stress, diffusion and the kinetics of nucleation combine in heteroepitaxial growth to form complex morphologies that include the formation of pits.
- These morphologies can be understood by quantifying the effect that inhomogeneities on the surface play in the process of pit nucleation.

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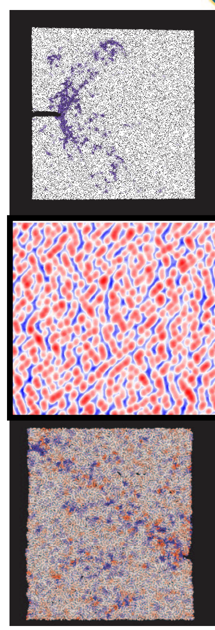

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