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Predictive Science for Stress Engineering at the Nanoscale

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National Nuclear Security Administration

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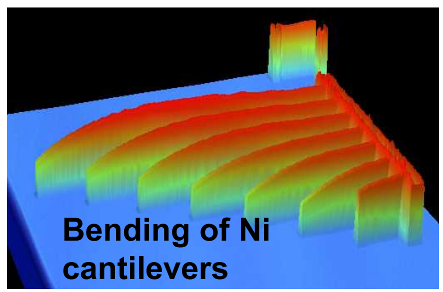
Sandia National Laboratories

Why Stress in Small Structures?

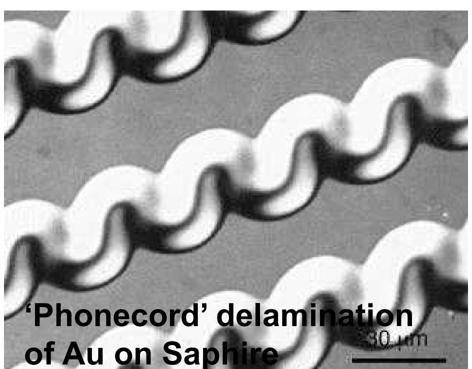
- Stress in supported structures and thin films strongly influences system behavior

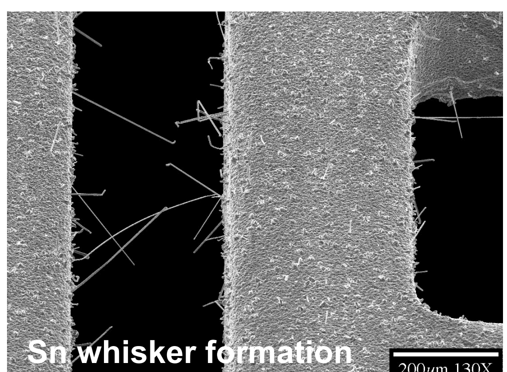
- Correlation between growth morphology and stress evolution unclear

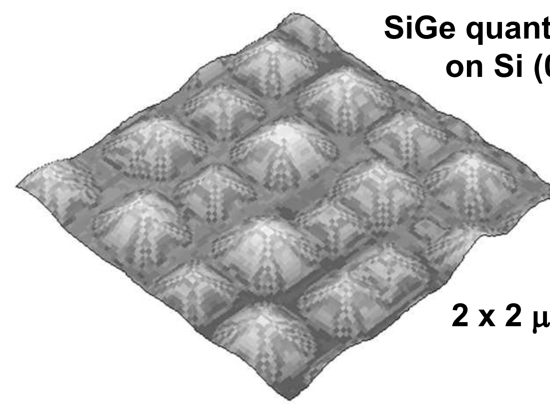
- Failure ….



- Success ….



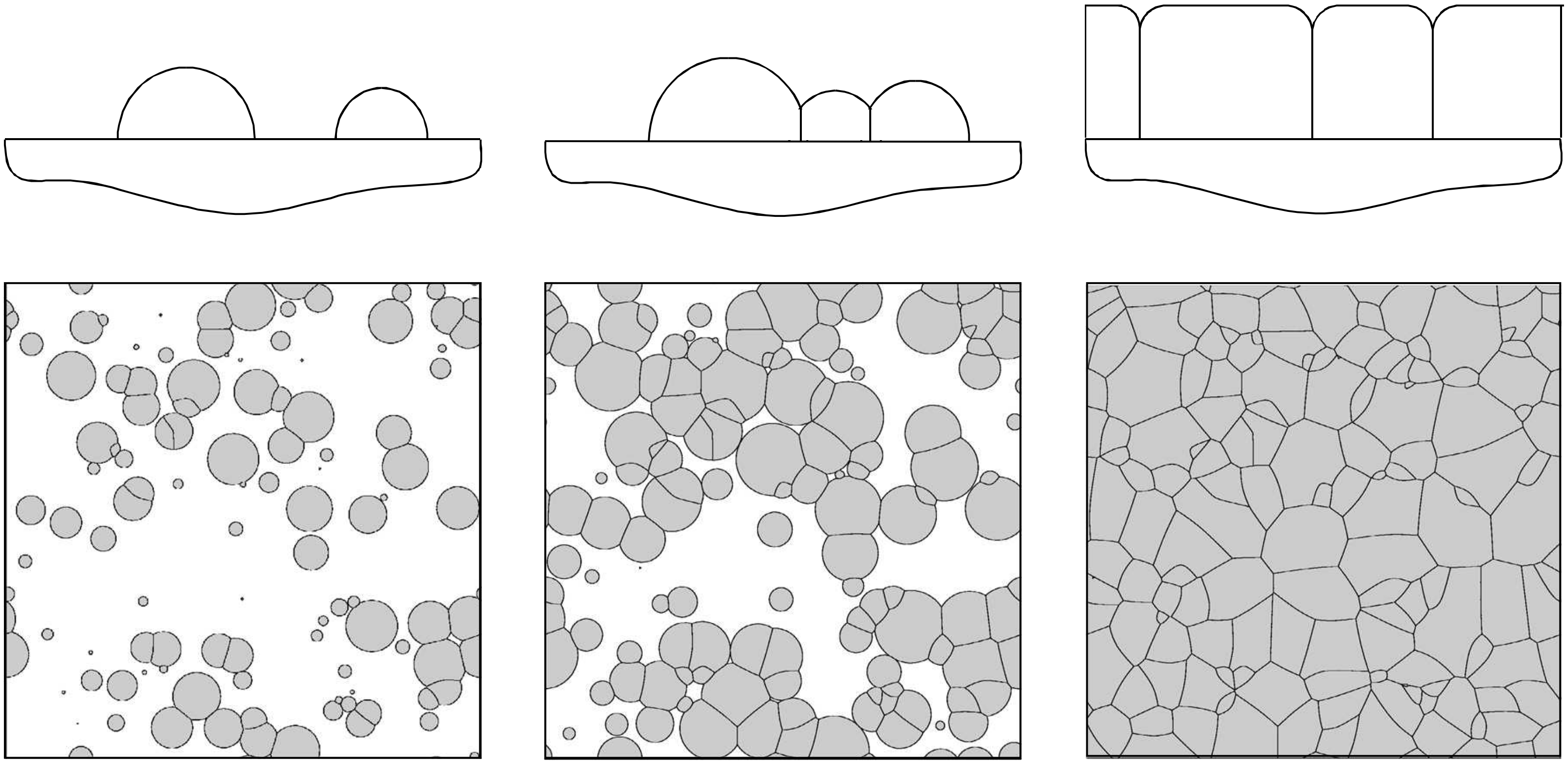




SiGe quantum dots on Si (001).

2 x 2 μm

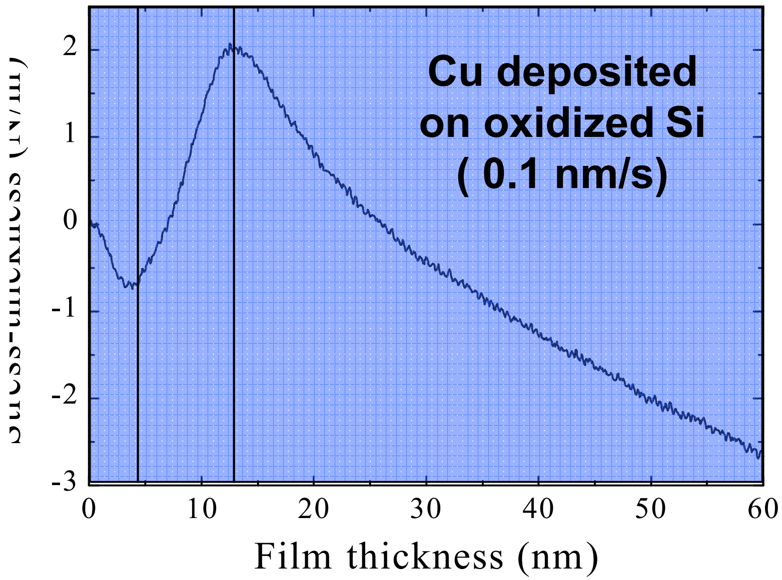
Volmer-Weber Thin Film Growth



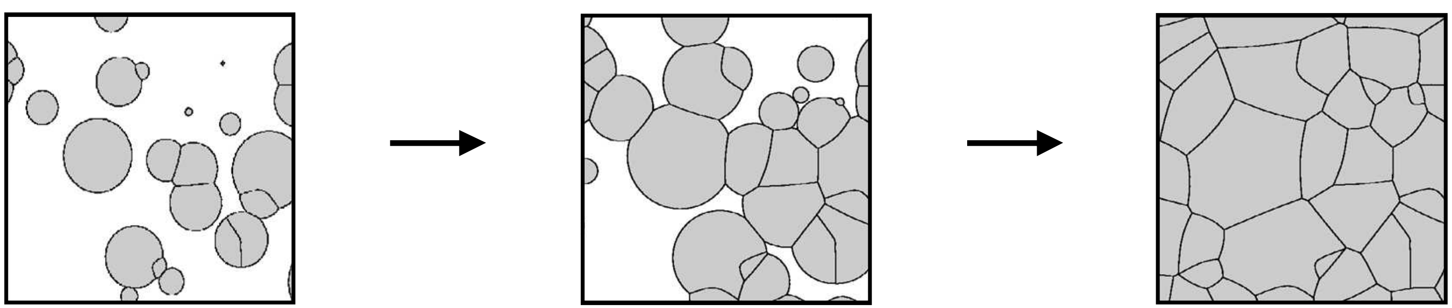
island nucleation → growth to impingement → film continuity

** exhibited by many material systems **

Stress During VW Growth

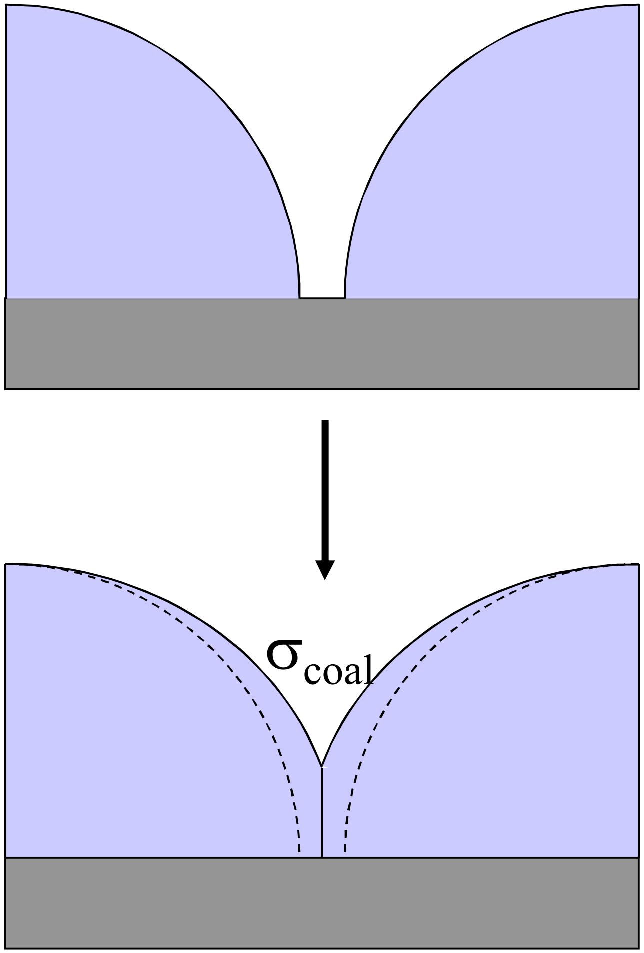


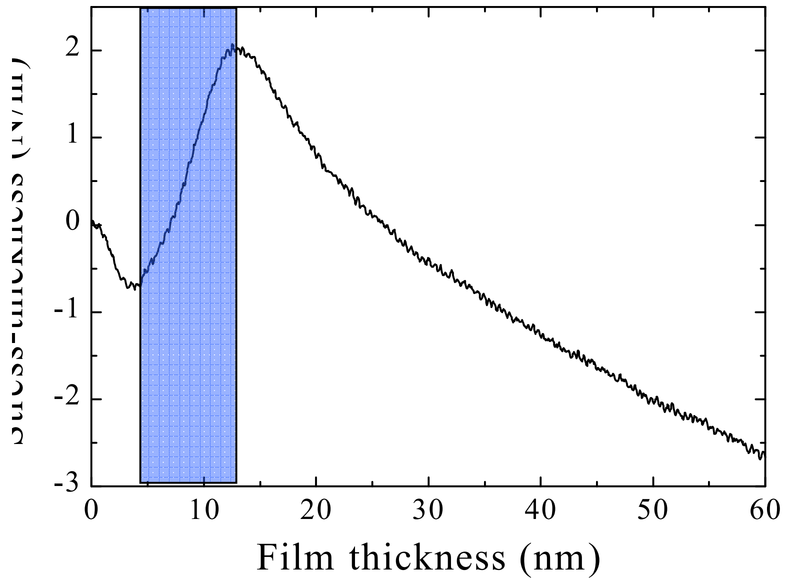
- Isolated islands (compressive stress)
- Island coalescence (tensile stress)
- Grain boundary formation (compressive stress)



island nucleation **island impingement** **film continuity**

Stress Evolution Theory: 2nd Growth Stage

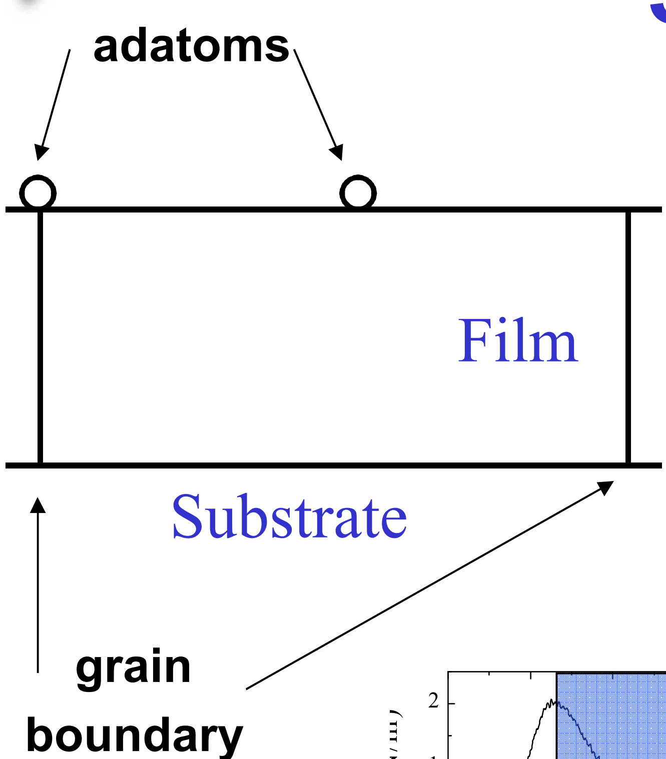


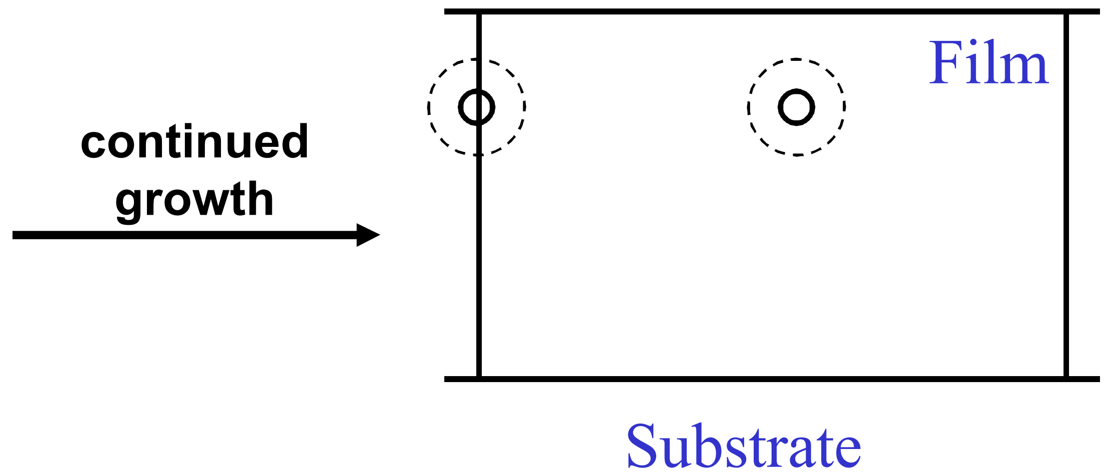


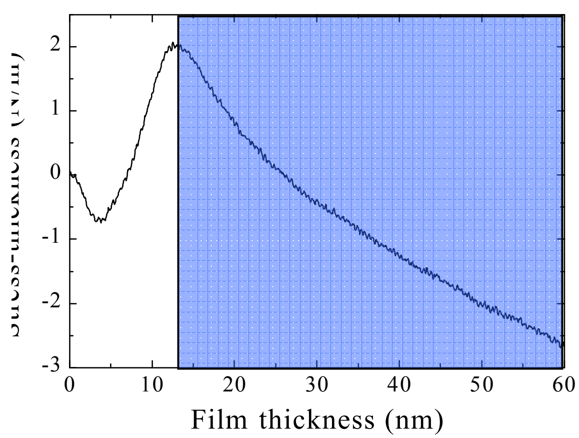
• Islands coalesce, reducing surface energy at the cost of generating elastic energy

• Evolution of tensile stress during 2nd growth stage

Stress Evolution Theory: 3rd Growth Stage

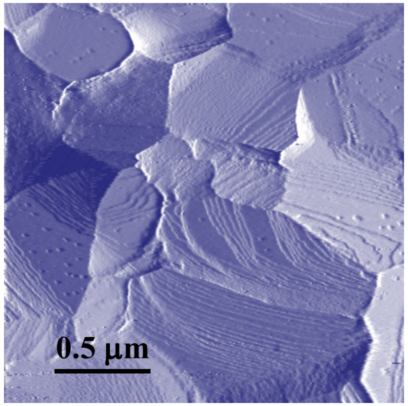




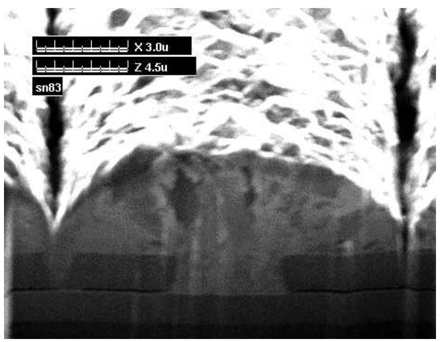


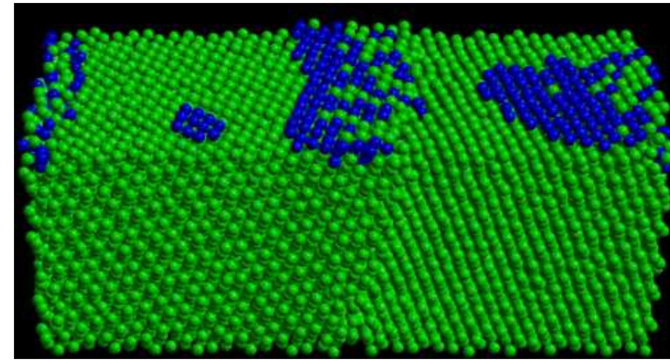
- Adatoms are trapped as grain boundary and/or bulk interstitials
- Evolution of compressive stress during 3rd growth stage

Studying Stress Evolution



Experiments



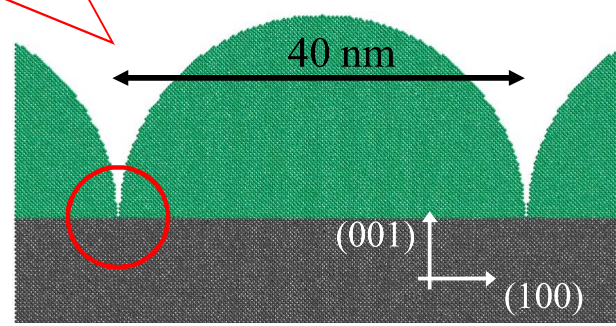


Atomistic Simulation

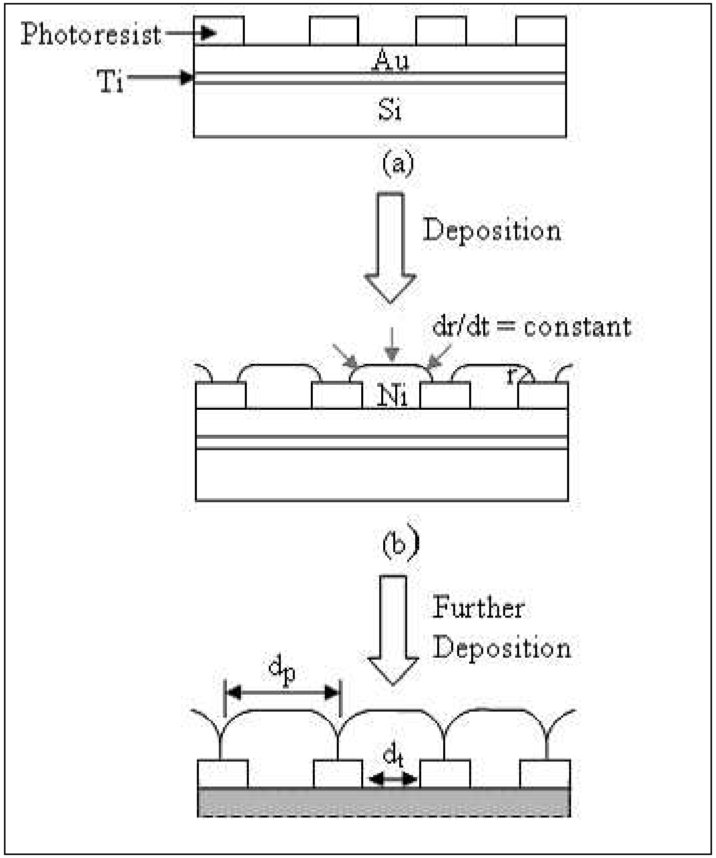
Multifaceted Study

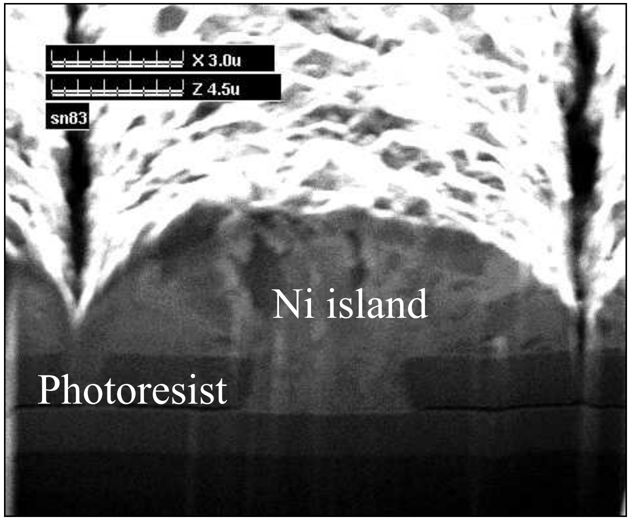
Analytical Modeling

$$\Delta E(\delta) = \frac{1}{2} M w \left(\frac{\alpha - \delta}{w} \right)^2 + \sigma_{pre} \cdot (\alpha - \delta) + \left[\gamma_i(\delta) - \gamma_i(\alpha) \right]$$



Growth Stress Evolution: Experiments



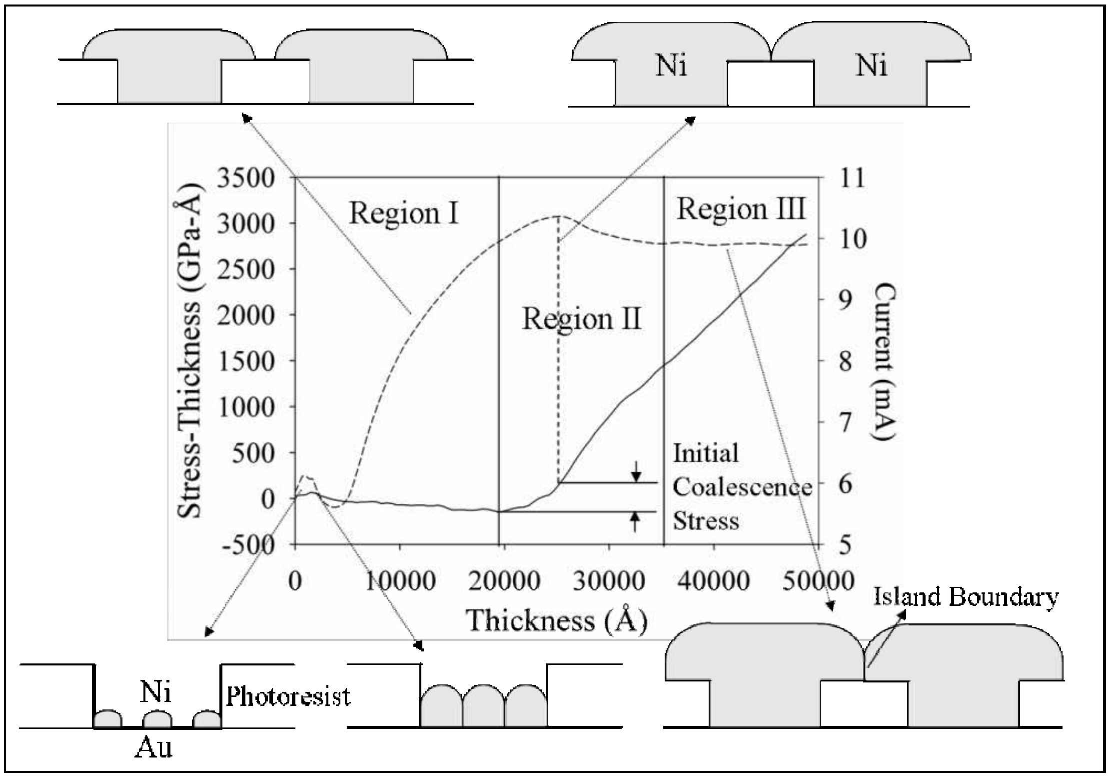


10.6 μm island, pre-coalescence

- Selective growth into patterned trenches permits highly controlled morphology during stress measurements
- Quantitatively determine morphology/stress relations

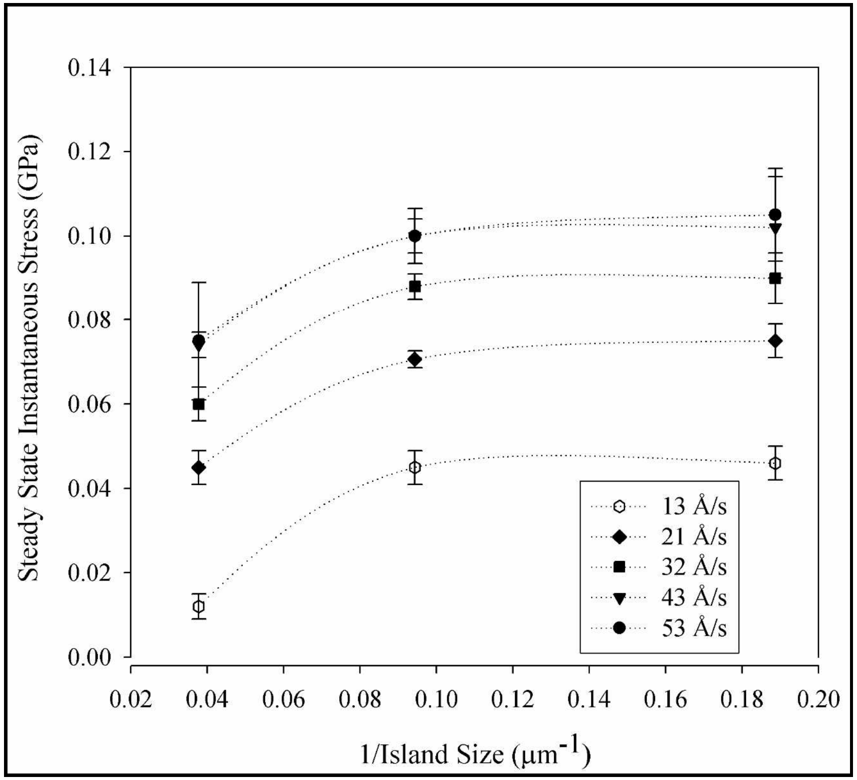
Initial vs. Ongoing Coalescence

• Simultaneous film stress and electrodeposition current measurements directly connect film morphology to stress



• Prior experiments could not distinguish tensile stress due to *initial* coalescence events from *ongoing* coalescence as a film planarizes

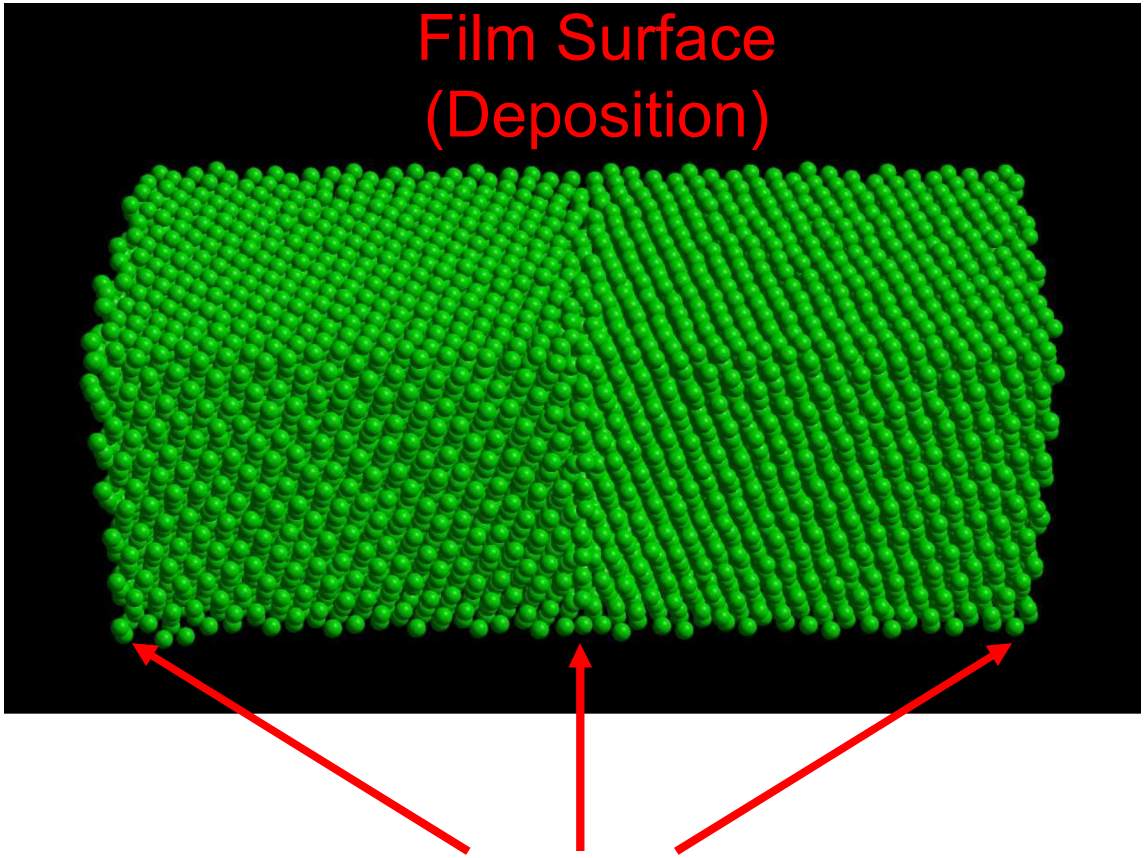
Competing Stress Generation Mechanisms



- Vary island size and deposition rate to examine geometry and kinetic effects during selective area growth experiments

There is a yield stress, geometry limited coalescence stress mechanism (tensile) that competes with a kinetically limited compressive stress generation mechanism (accepted for publication, *JAP*).

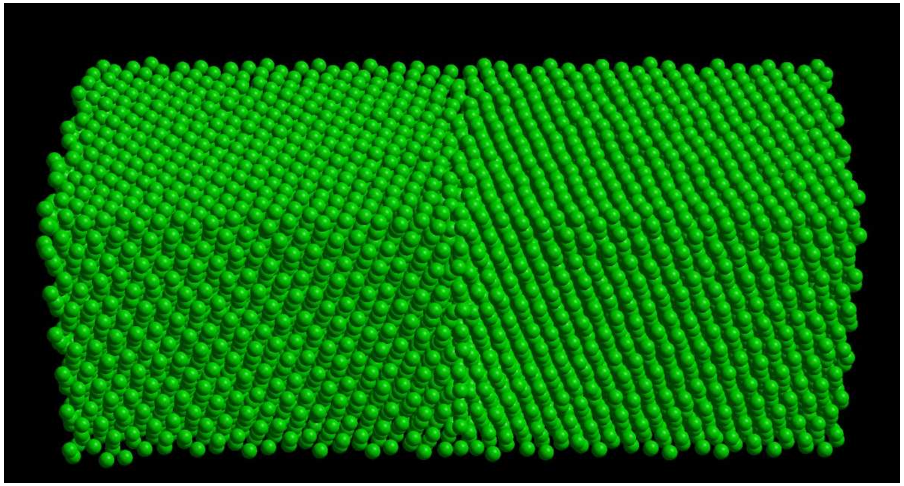
Late Stage Compressive Stress Evolution: Simulation



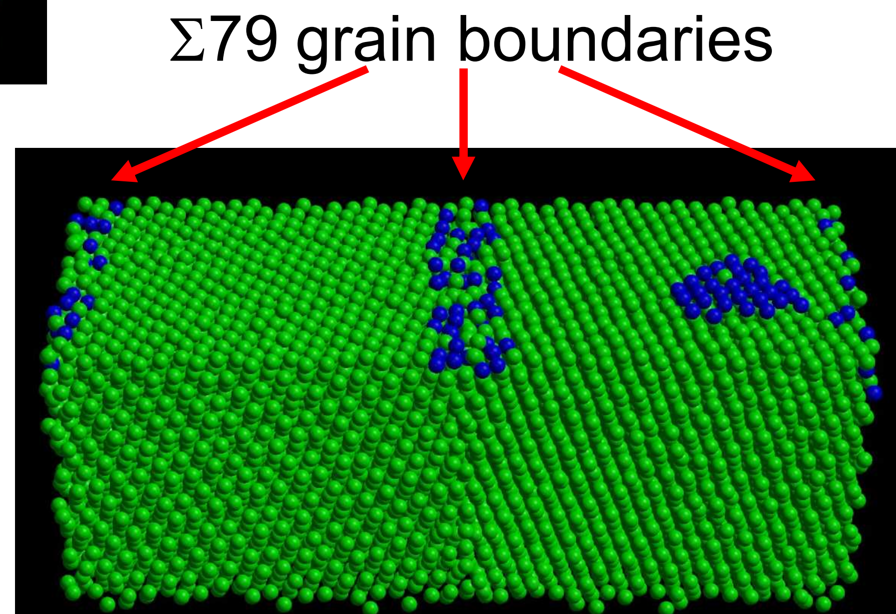
Σ79 grain boundaries

- **Deposit atoms onto free surface of film intersected by grain boundaries**
- **fixed at bottom (mimics film growth)**
- **~0.4 monolayers deposited**

Late Stage Compressive Stress Evolution: Simulation

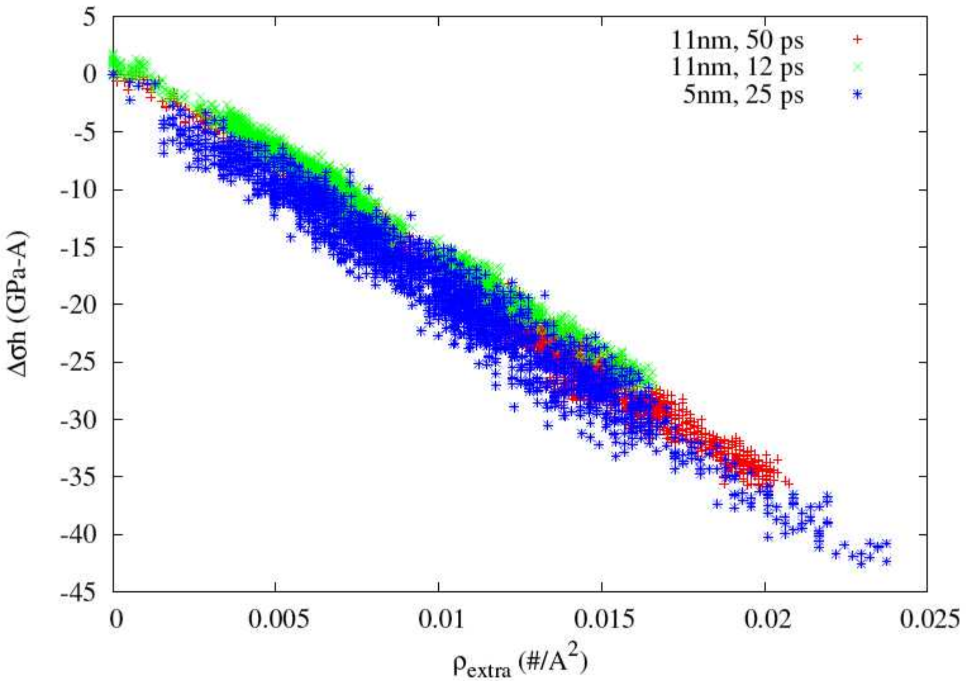


• Ni adatoms (blue) on Ni (111) film (green) intersected by Σ79 grain boundary



• First simulations demonstrating adatom incorporation near grain boundary

Late Stage Compressive Stress Evolution: Simulation



• Adatom incorporation near grain boundaries directly correlates with compressive stress evolution

• Atomic scale calculations permit us to quantitatively understand the kinetically limited compressive stress generation mechanism

• *Suggest ways to 'tune' stress state in growing metal systems*

Conclusions and Outlook

- Addressing *grand challenges* in stress evolution during thin film growth

- Meeting a complex, multifaceted set of unknowns by leveraging a unique combination of skills and tools

- Eyes on the prize … proactive approach in MS&T to make possible predictive capability for engineering stress during materials growth

- A concluding exercise of the project will be to identify steps necessary to turn new materials models for stress evolution into a ***predictive engineering tool***