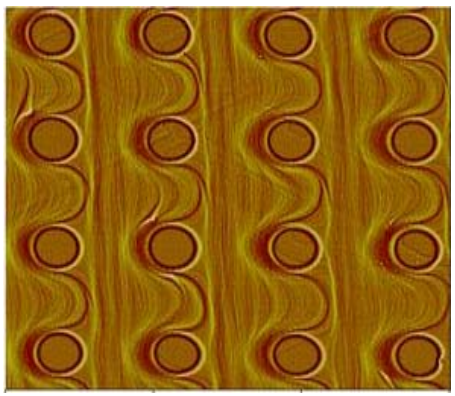
Length Scales in Step-Bunch Self-Organization during Annealing of Patterned Vicinal Si(111) Surfaces

T. Kwon, H.-C. Kan, and R. J. Phaneuf

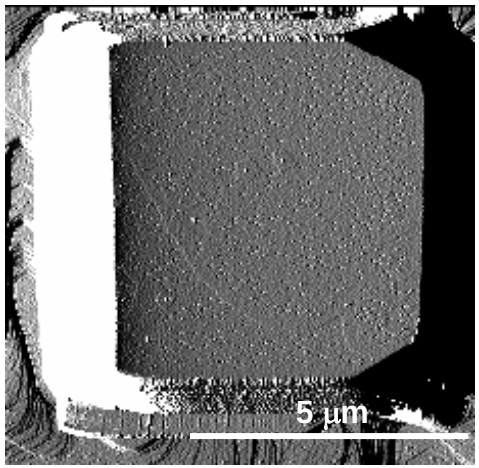


Nonequilibrium Interface and Surface Dynamics: Theory, Experiment and Simulation from Atomistic to Continuum Scales

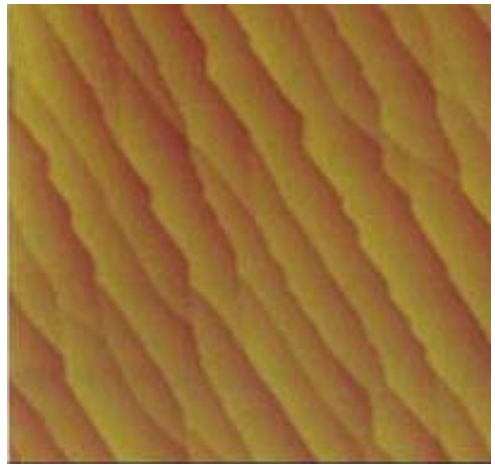
CSCAMM, April 23, 2007

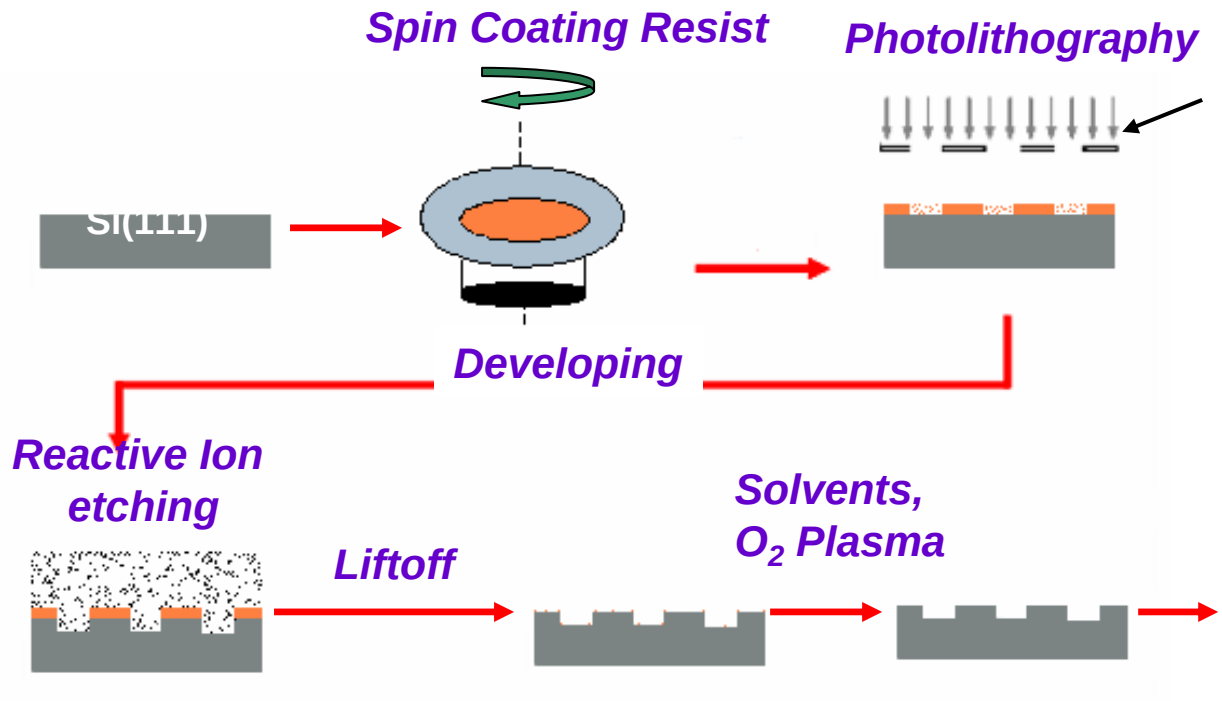
The Laboratory for Physical Sciences

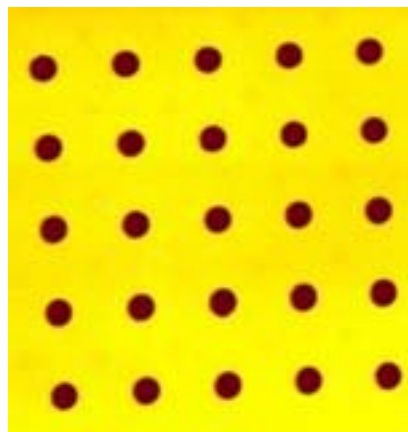
Silicon Surfaces – *Flat, Stepped & Patterned*



D. Lee, et al., MRS Sym Proc. 648 (2001)

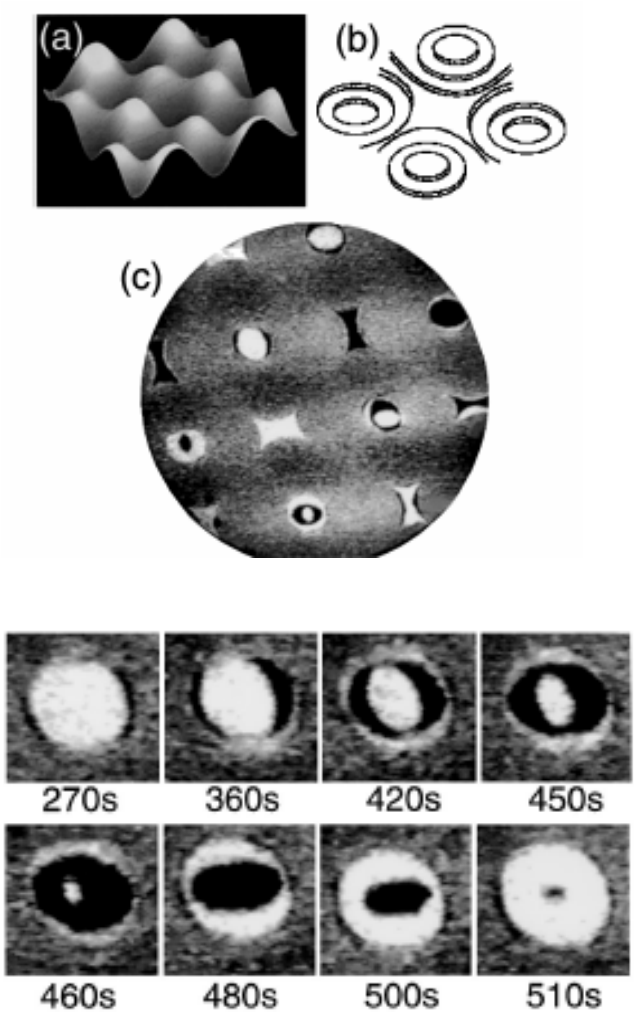






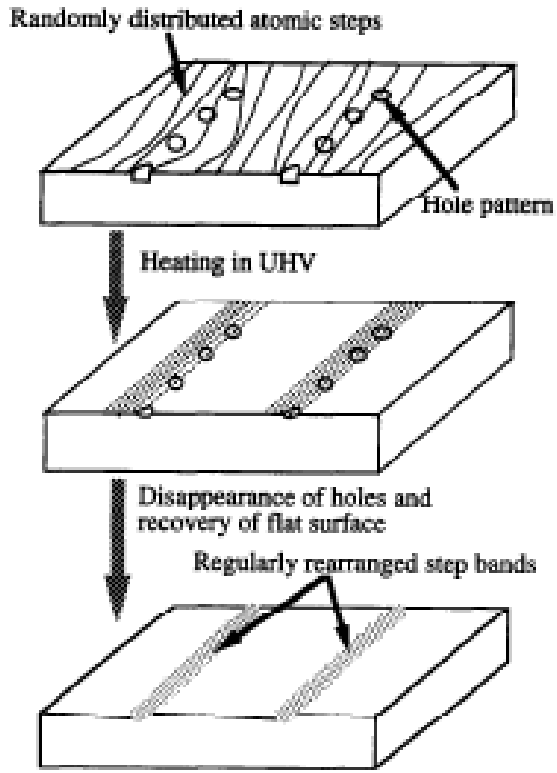
Patterned Silicon Surfaces – *Relaxation Kinetics*

Relaxation of Patterned Si(001)



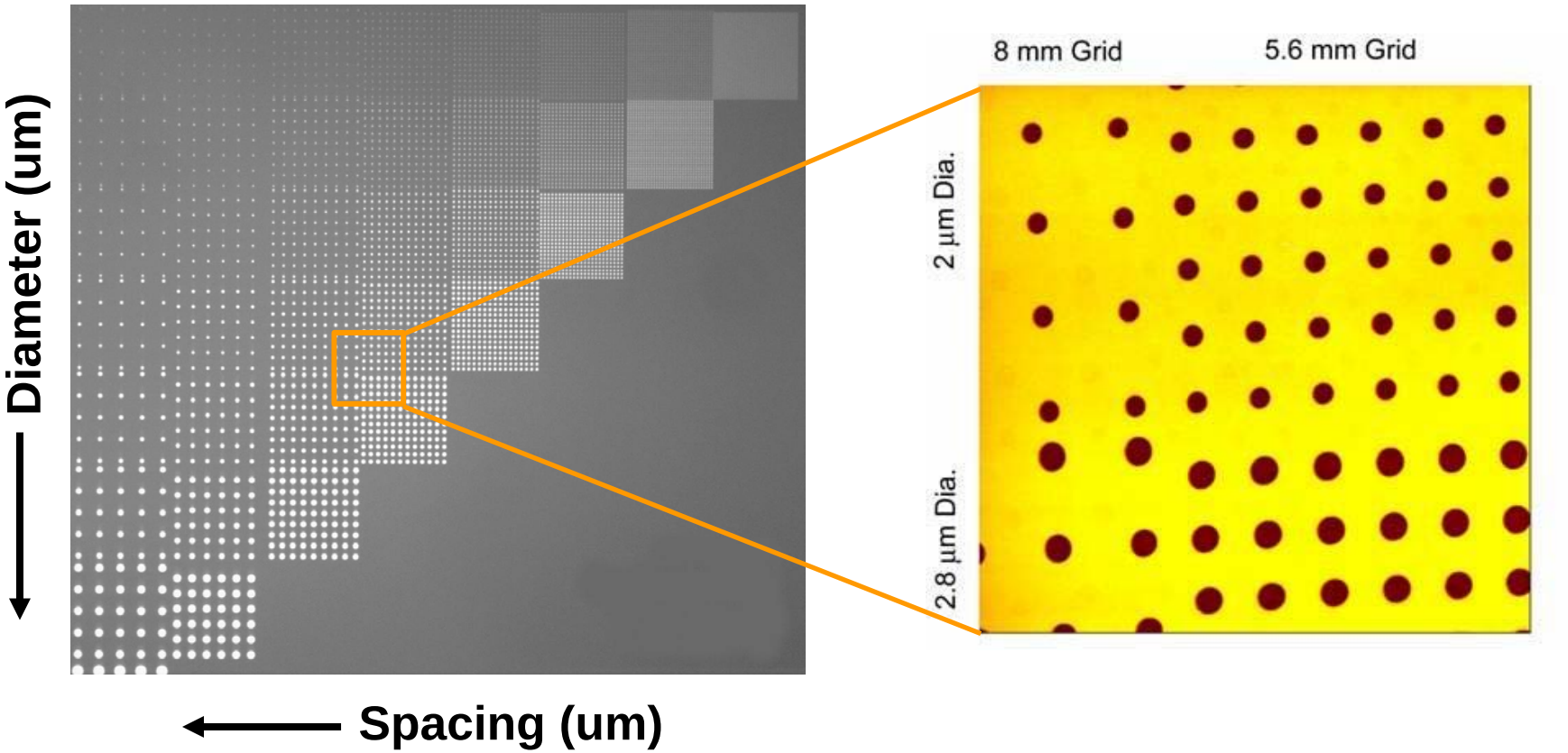
S. Tanaka, et al, PRL 78, 3342 (1997)

Annealing of Patterned Vicinal Si(111)



T. Ogino, Surf. Sci 386, 137 (1997)

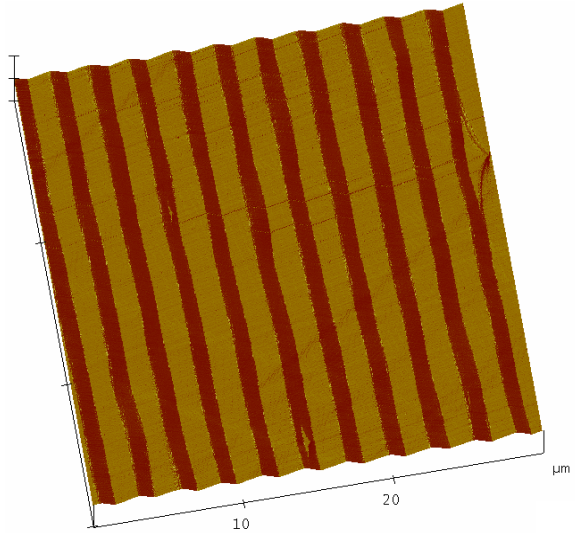
Lithographically Patterned Surface – *Combinatorial Length Scale Investigation*



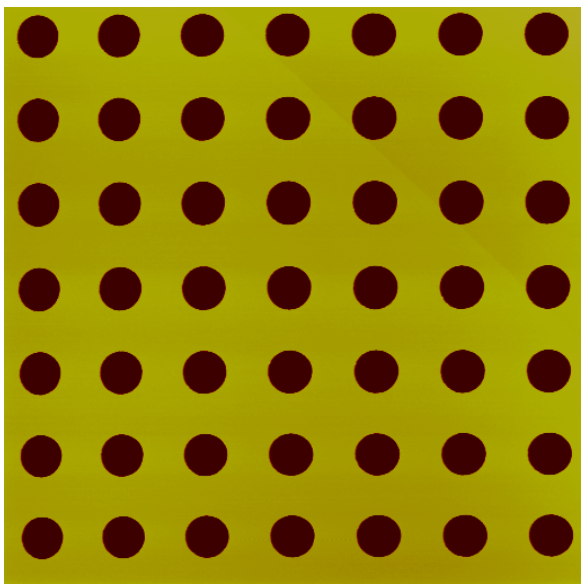
Effect of Annealing (1273 ºC)

Small Period Limit – *1.4 μm*

Diameter x 2.8 μm Pitch



Before Anneal



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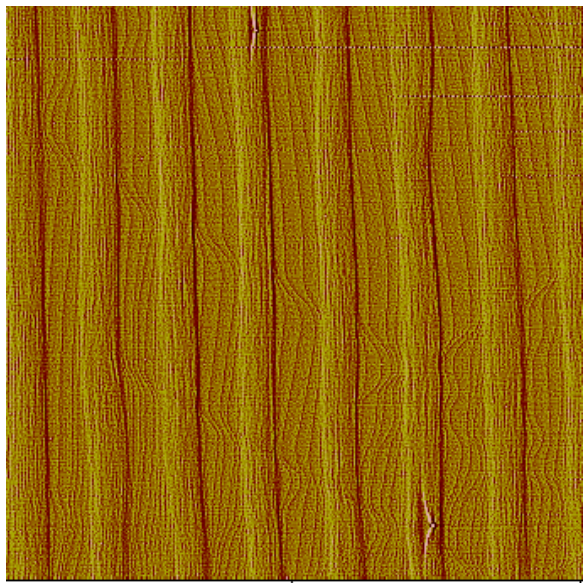
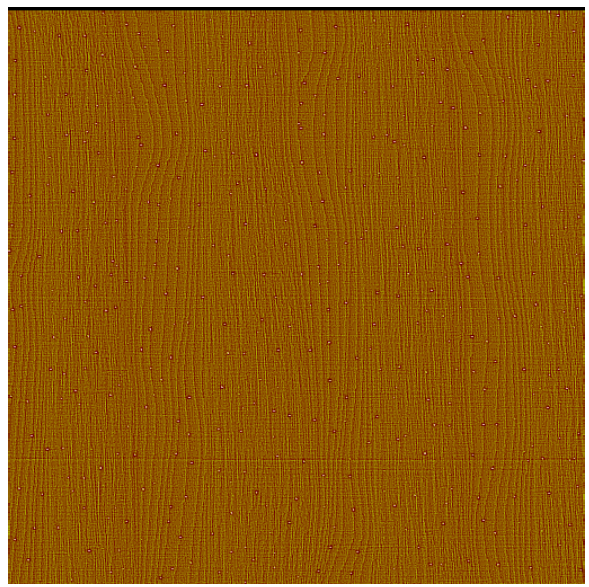
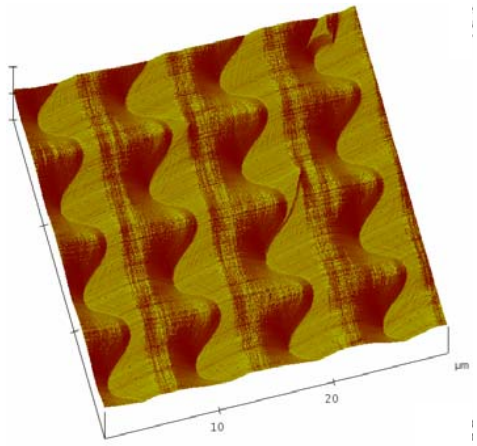


t = 65 s

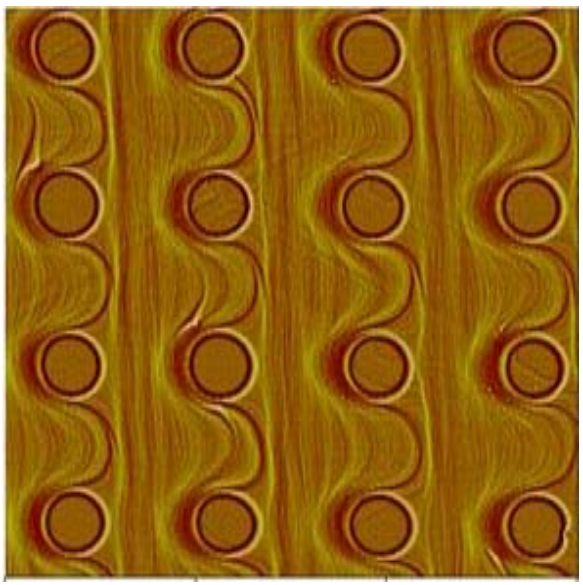


⟵ Up hill Down hill ⟶

Effect of Annealing (1273 ºC) Intermediate Period Regime – *4 μm Diameter x 8 μm Pitch*

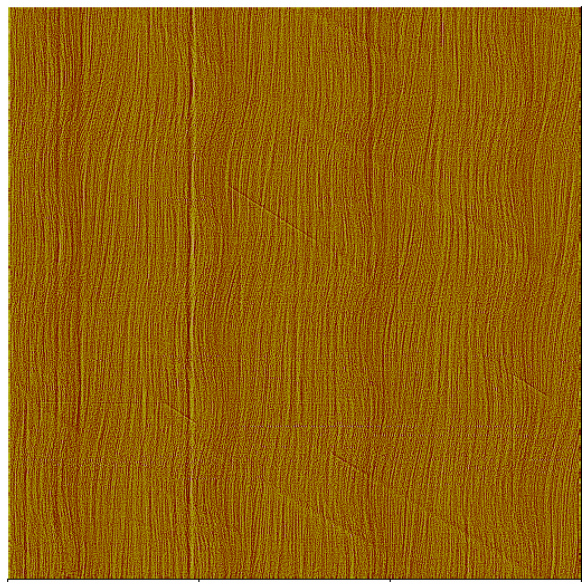


t = 30 s



t = 65 s

t = 2400 s

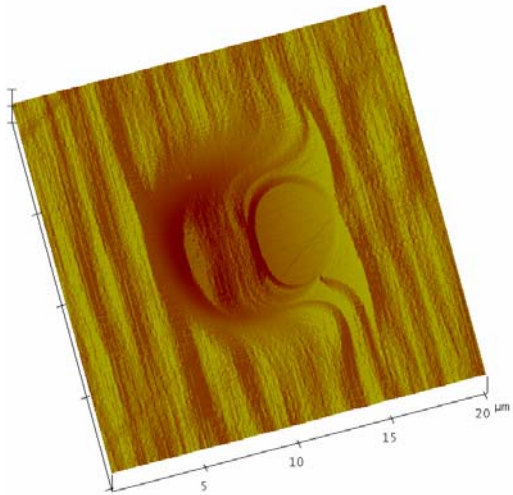


⟵ Up hill Down hill ⟶

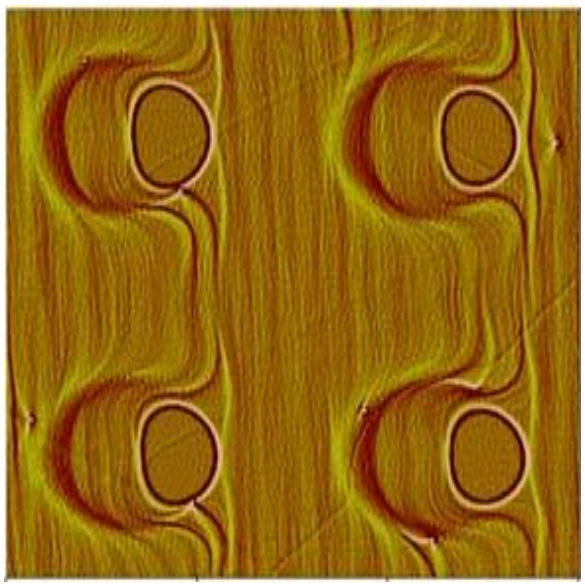
Effect of Annealing (1273 ºC)

Large Period Limit – *8 μm*

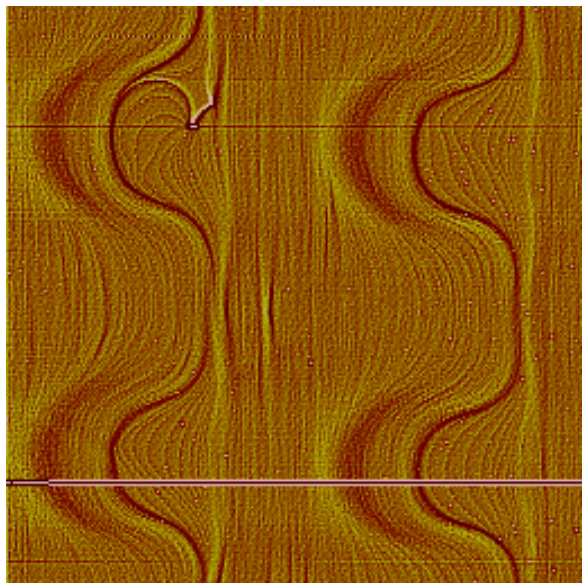
Diameter x 16 μm Pitch



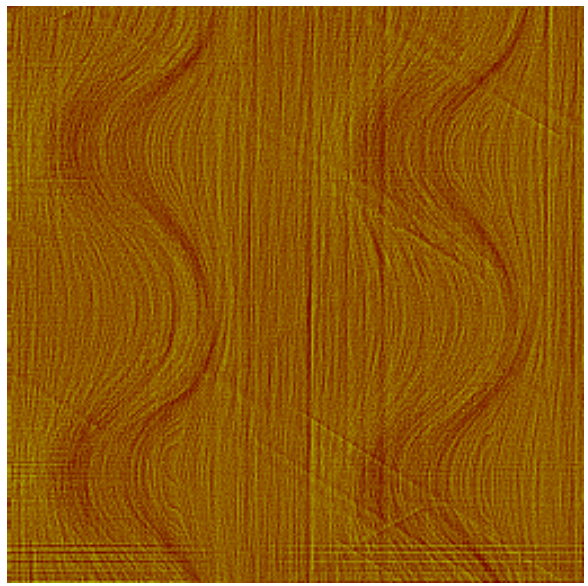
t = 30 s



t = 65 s



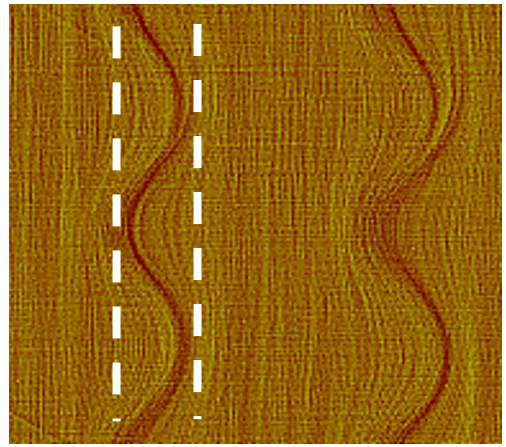
t = 2400 s

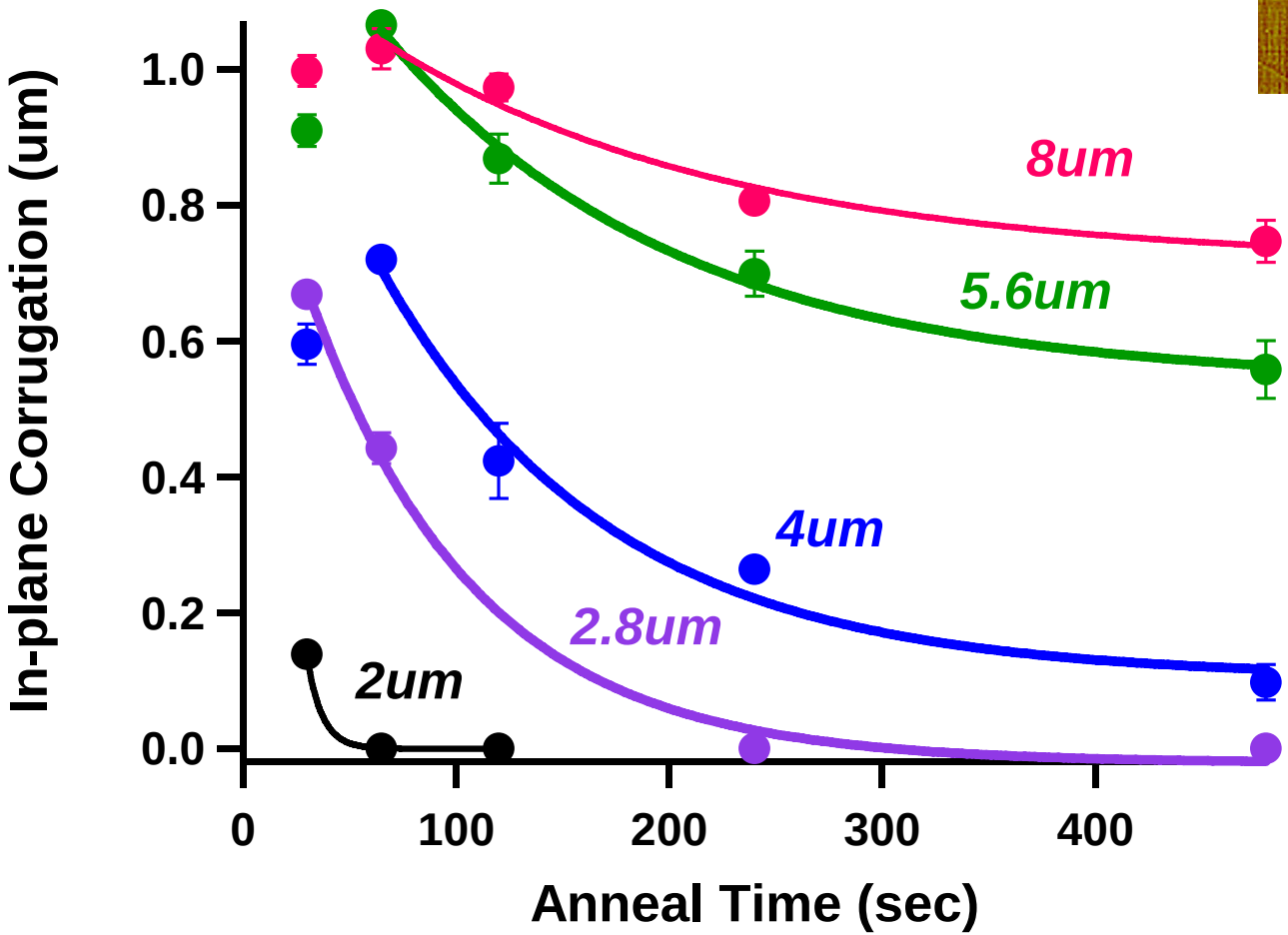


⟵ Up hill Down hill ⟶

In-Plane Corrugation – *Step Bunch*

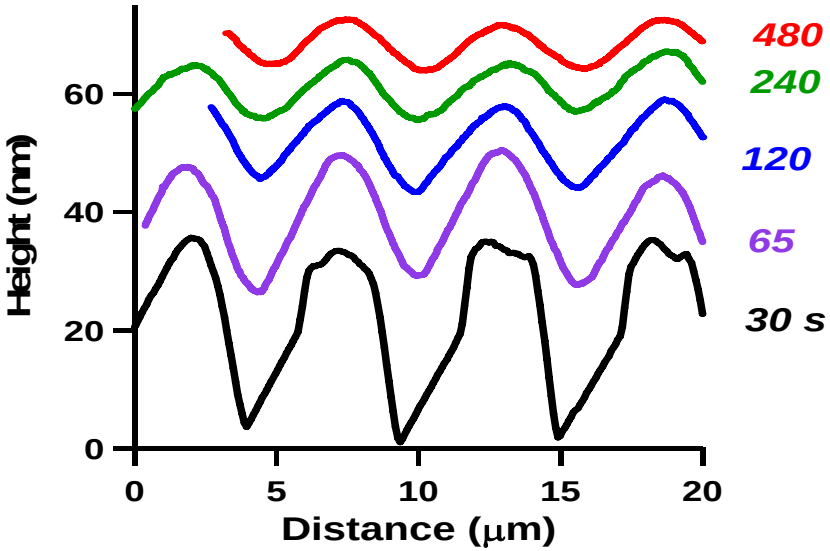
"Waviness"

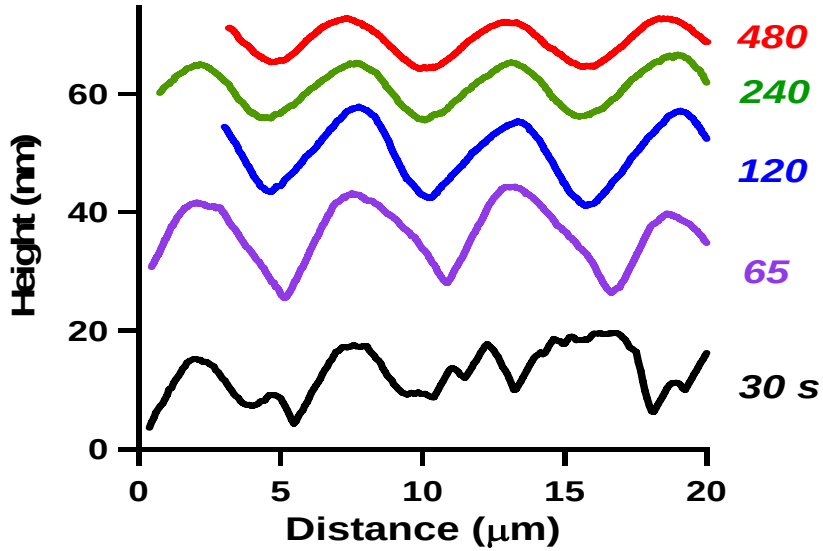


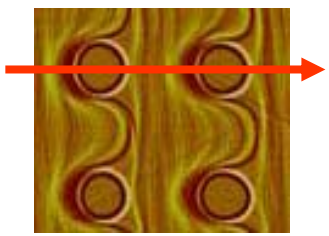


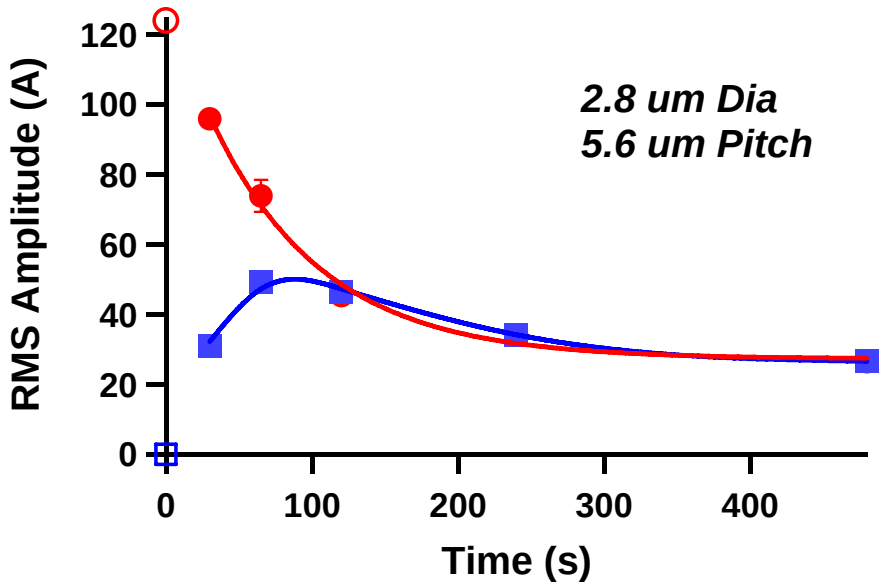
Out-of-Plane Corrugation- *Step Bunch Height*

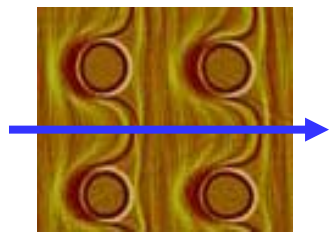
2.8 um Diameter x 5.6 um Spacing



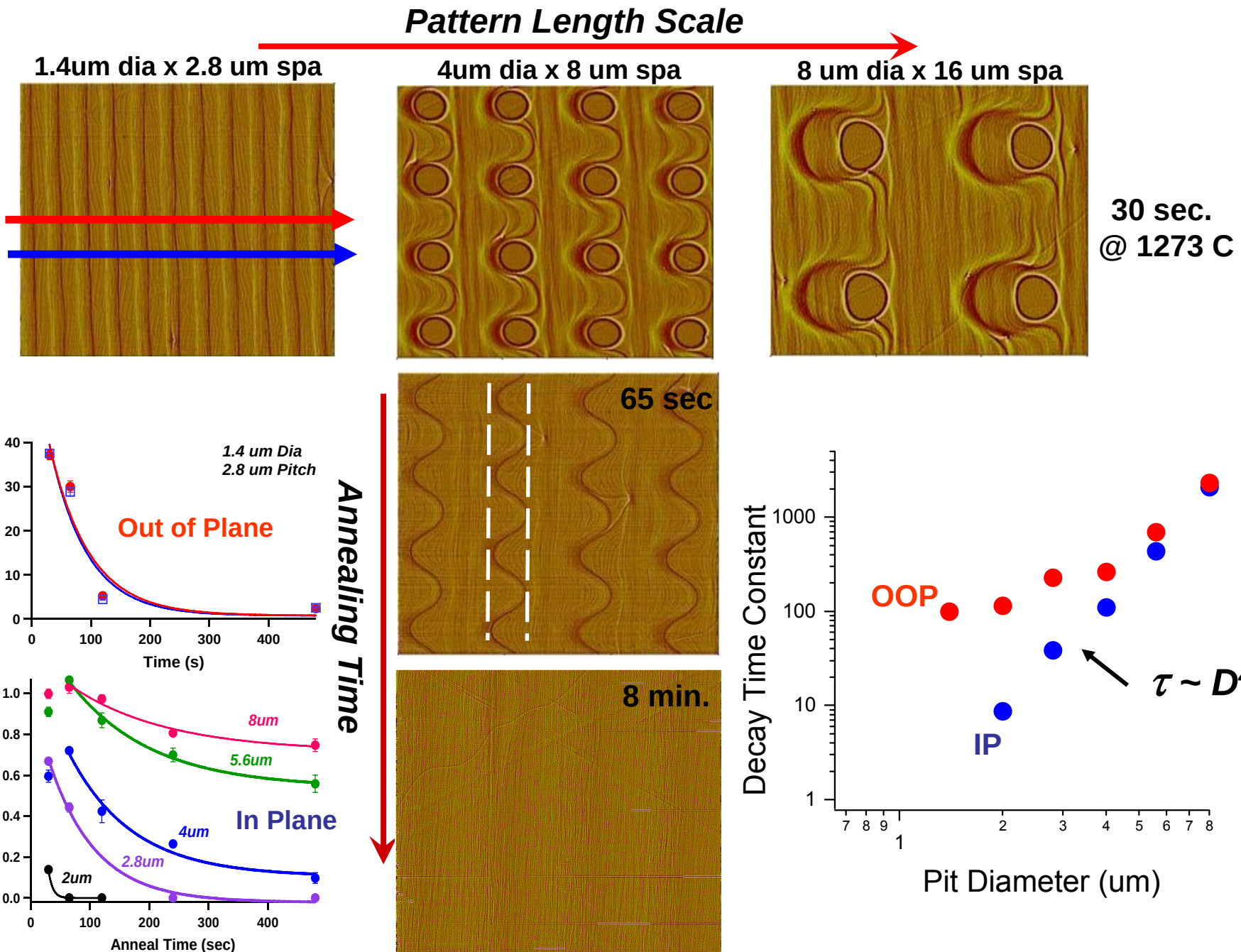




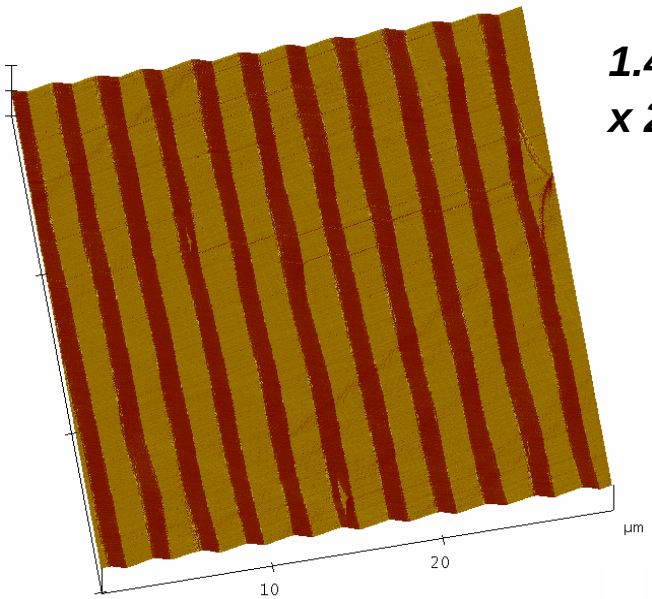




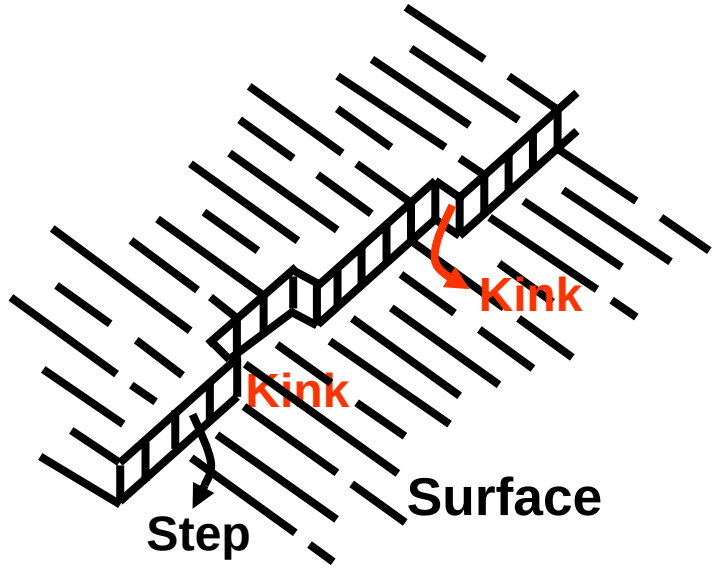
Evolution: Effects of length scale & Annealing time

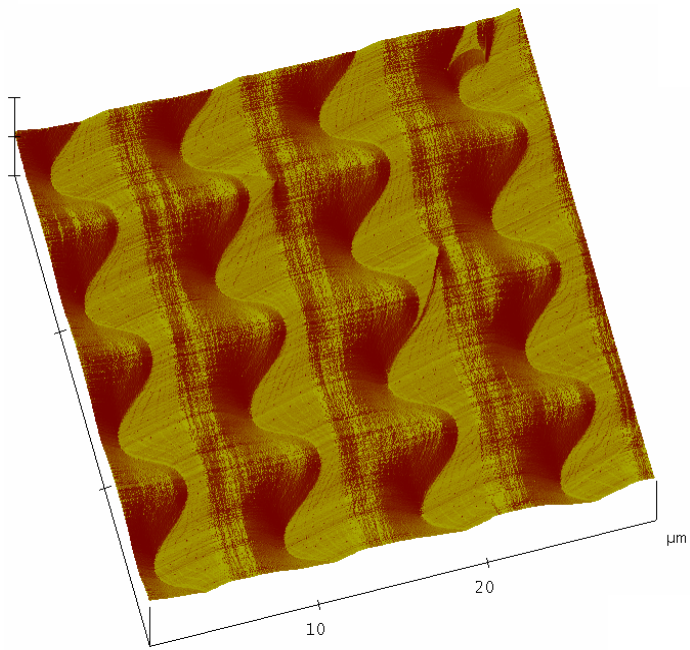


Step Stiffness- *Steps And Kinks Produce Extra Broken Bonds*



1.4 µm Diameter
x 2.8 µm Pitch





4 µm Diameter
X 8 µm Pitch

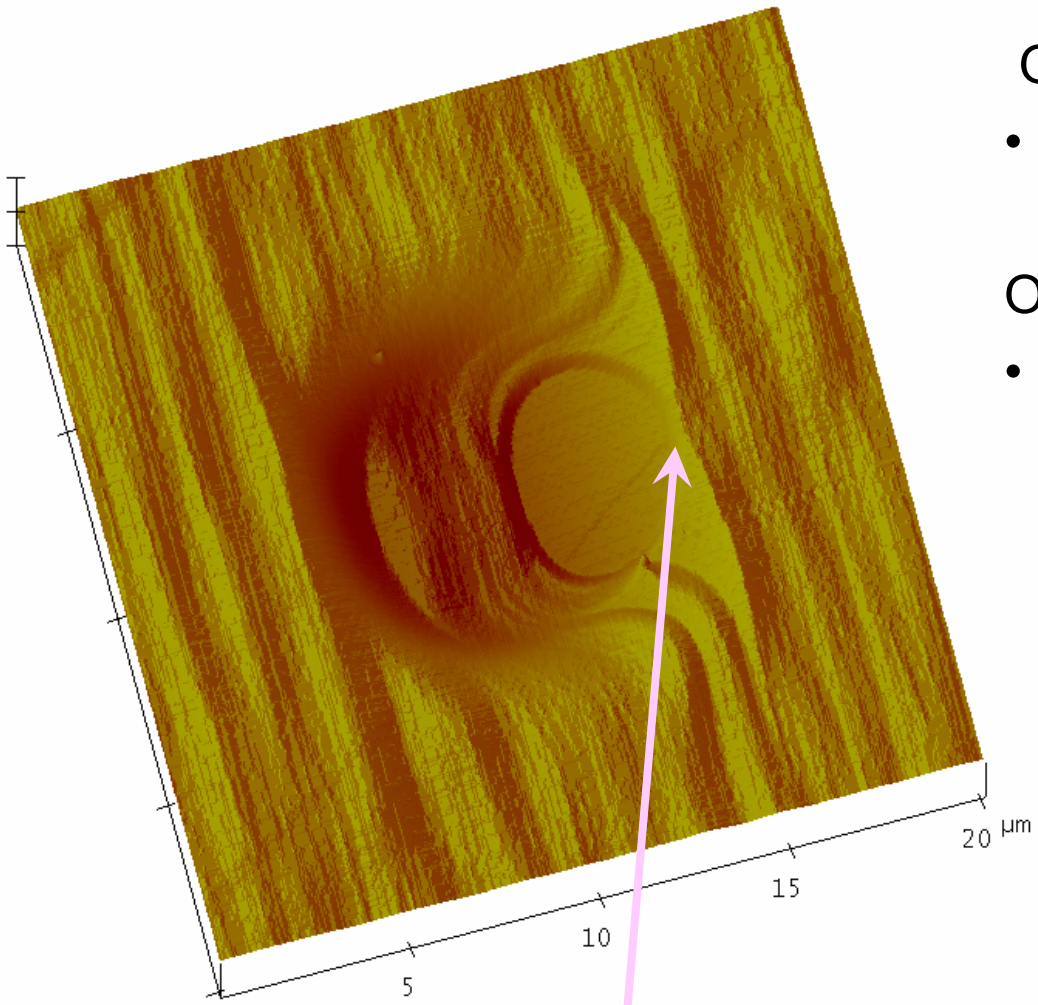
Free Energy/Area

$$f = f_0 + \frac{\beta}{l} + \frac{gh}{l^3}$$

$$\beta = \beta + \frac{\partial^2 \beta}{\partial \phi^2}$$

Step-Step Interaction –

8 μm Dia. x 16 μm Pitch : 30 sec. @ 1273 C



On uphill side of the pit,

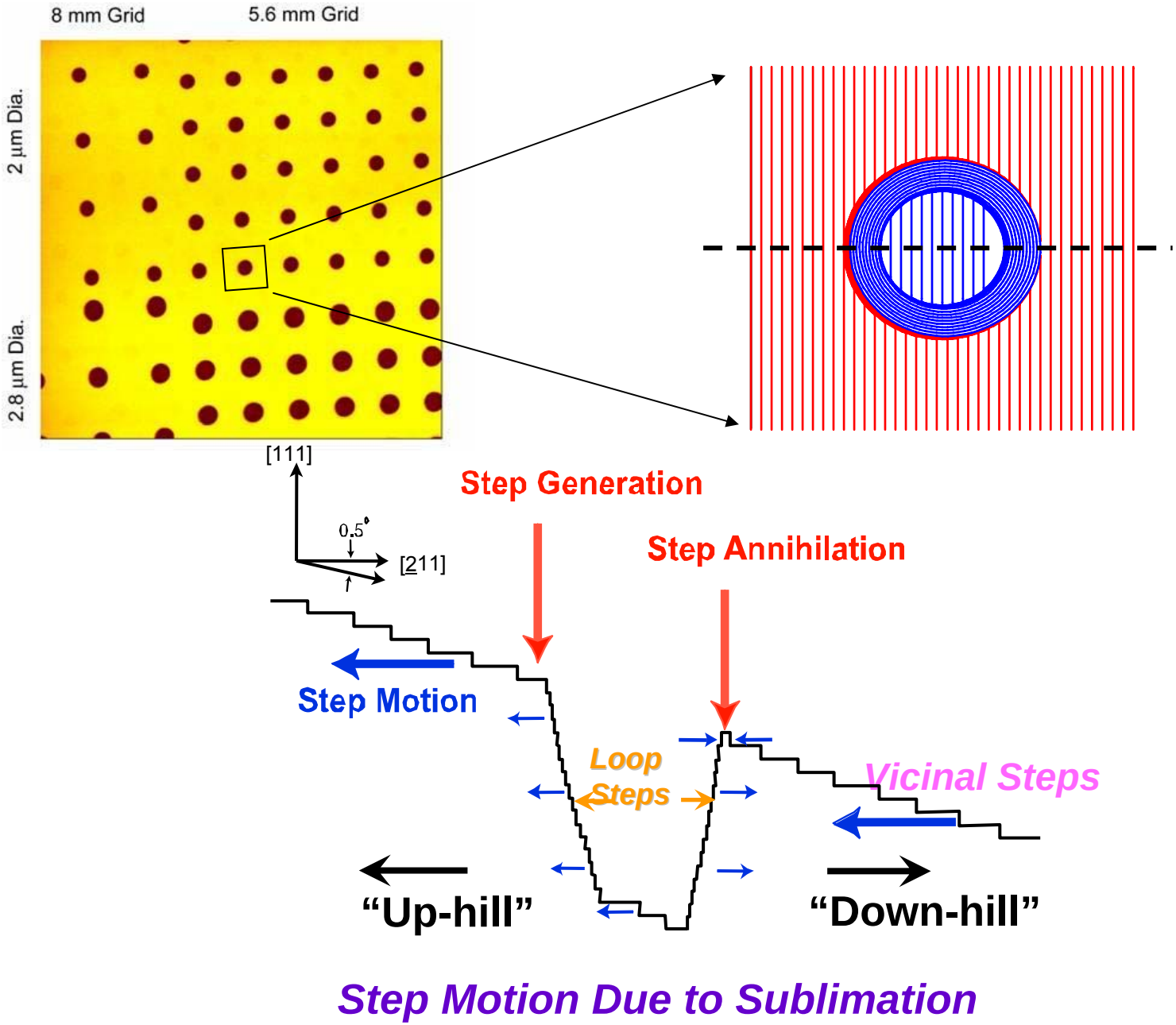
- Repulsive step-step interaction

On downhill side of the pit,

- **Bowed downhill wall**
  possible sign of ***attractive step-step interaction***

$$f = f_0 + \frac{\beta}{l} + \frac{gh}{l^3}$$

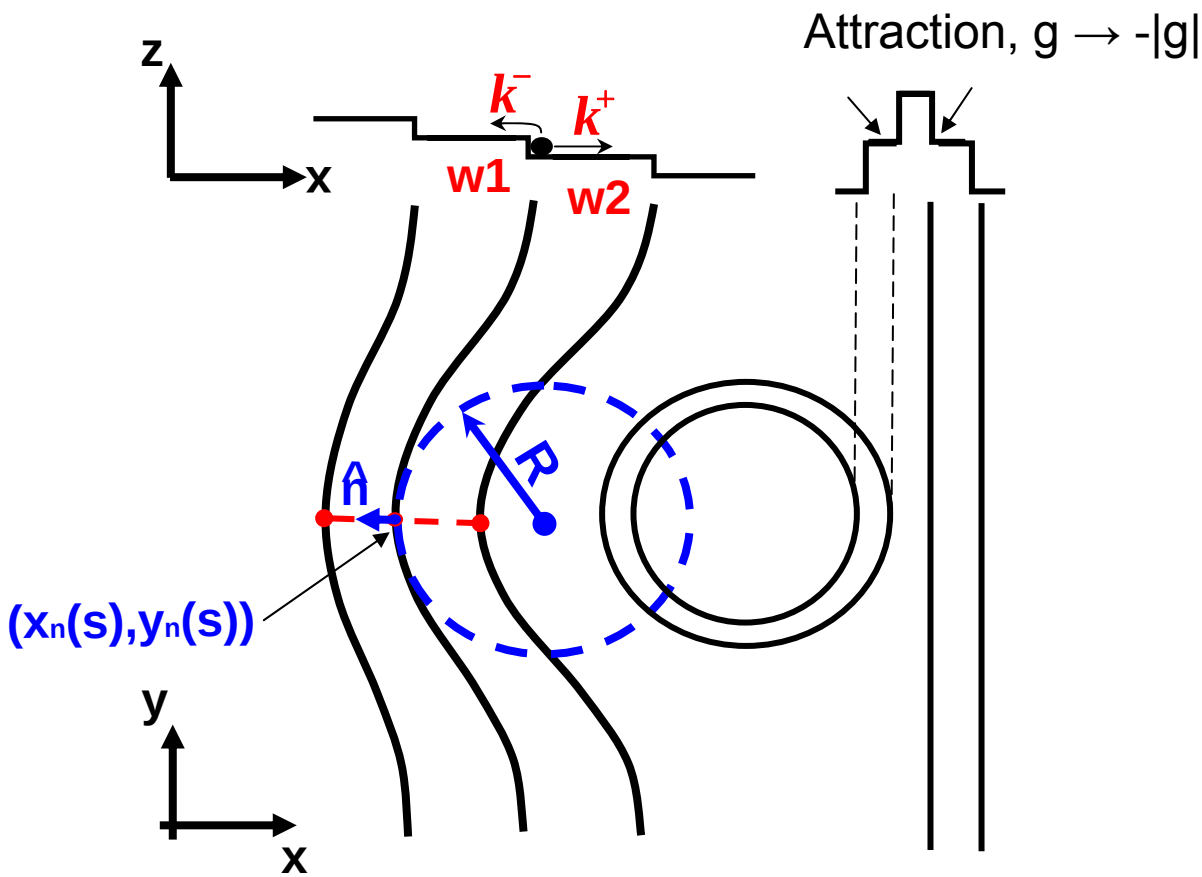
Step profile on a patterned vicinal surface



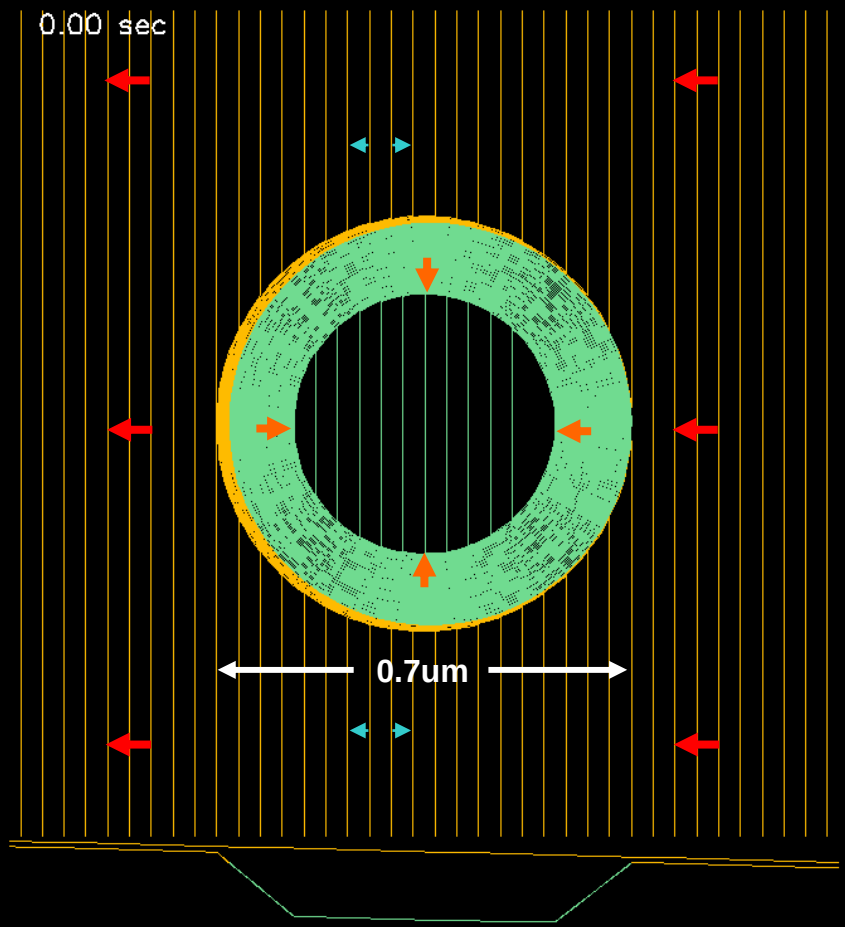
Step Motion Due to Sublimation

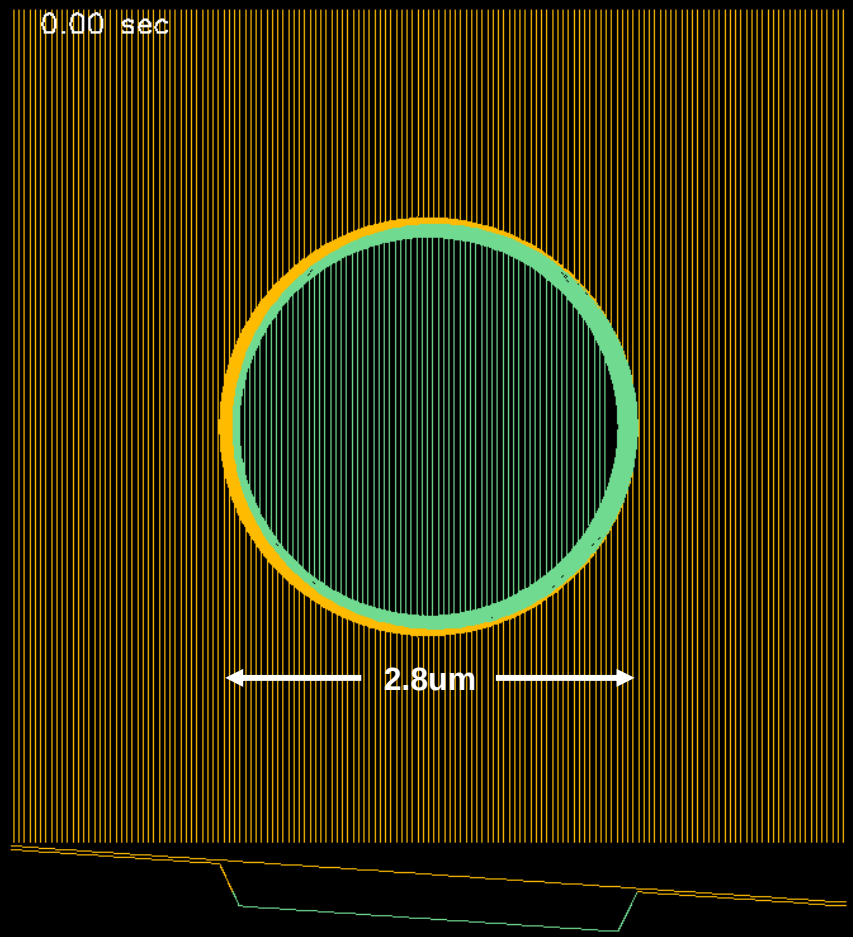
Mesoscopic Model for Step Kinetics*

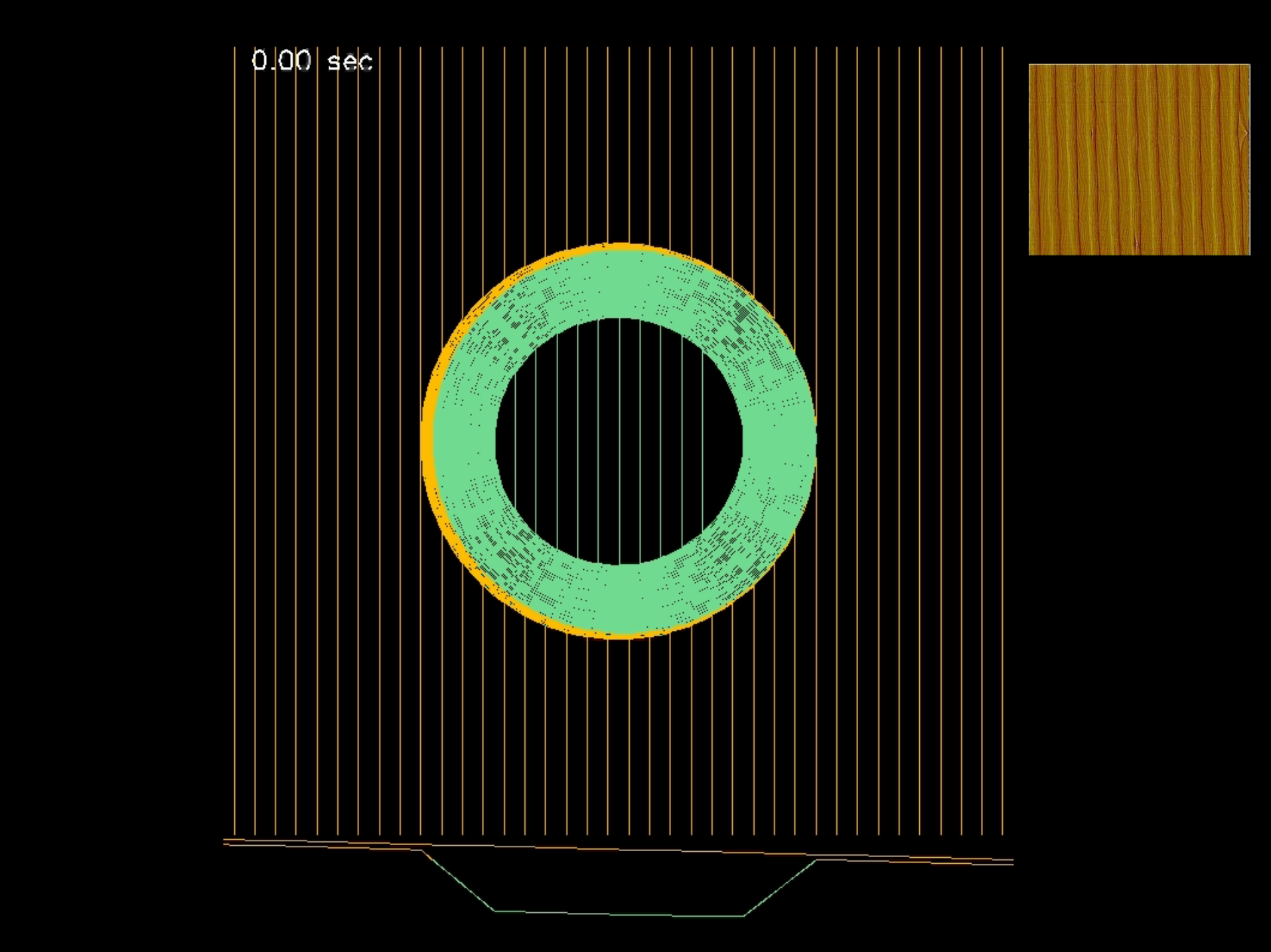
$$\frac{d\left(x_n, y_n\right)}{dt} = \frac{\Gamma}{kT}\left(\tilde{\beta} \cdot \frac{1}{R} + 2\,gh^{3} \cdot \left(\frac{1}{w_1^3} - \frac{1}{w_2^3} \right) \right) \cdot \hat{n} \; - \left(k^{+} \cdot w_2 + k^{-} \cdot w_1 \right) \cdot \hat{n}$$



*J.D. Weeks *et. al. "Dynamics o f Crystal Surfaces and Interfaces", Plenum Press 1996*


0.00 sec
0.7um


0.00 sec
2.8um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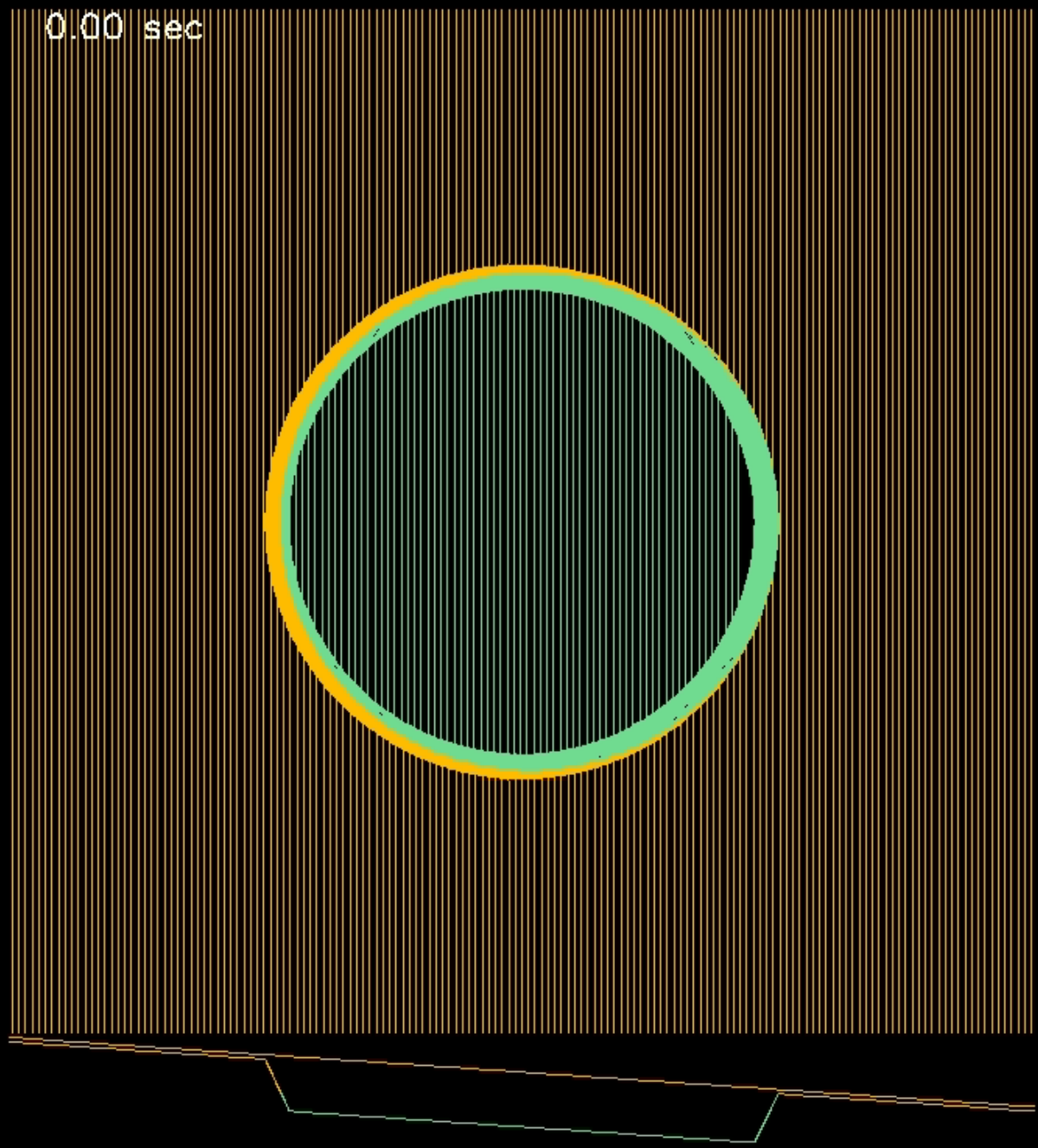
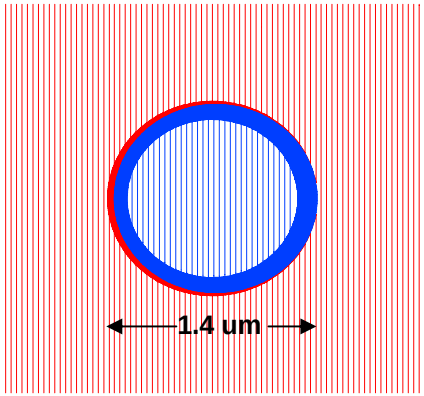
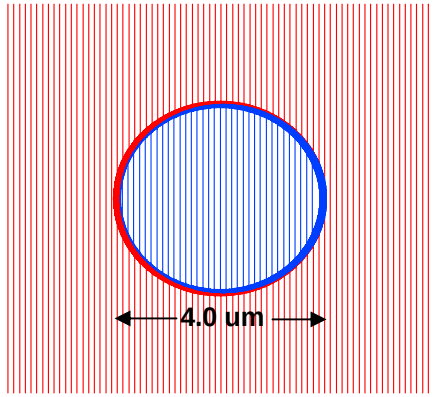
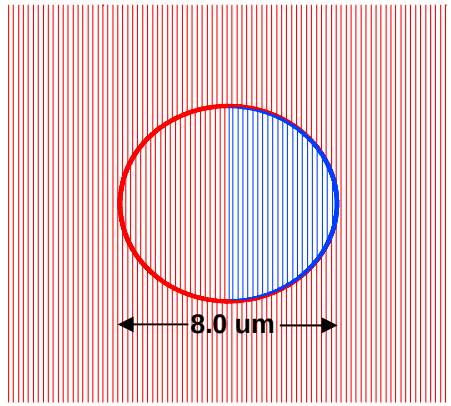

0.00 sec

Simulated Length scale dependence on Pit Evolution

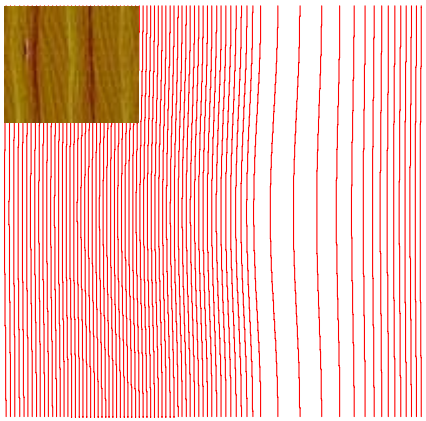
t=0s

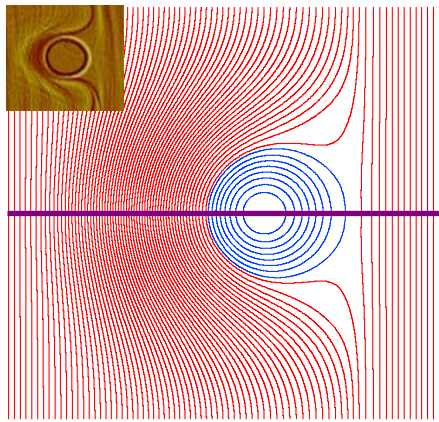


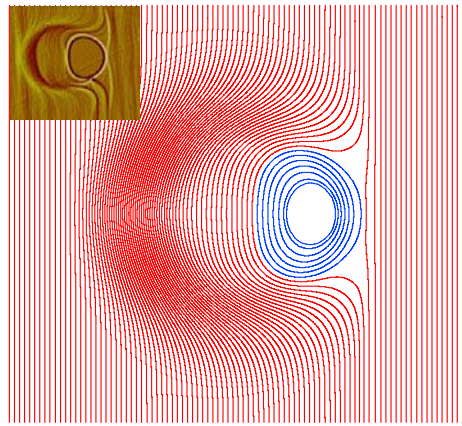


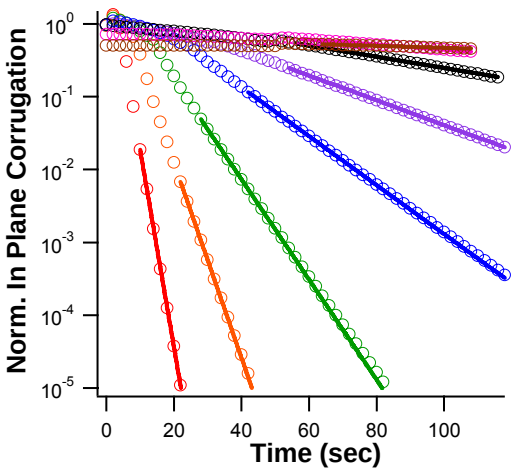


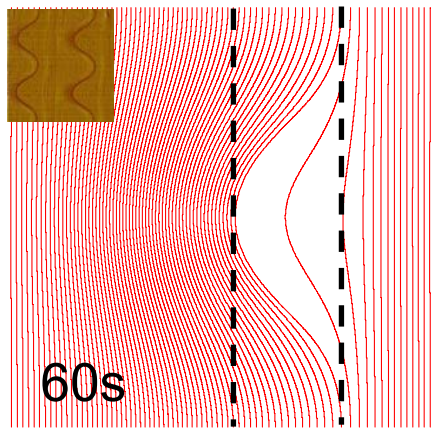
30s

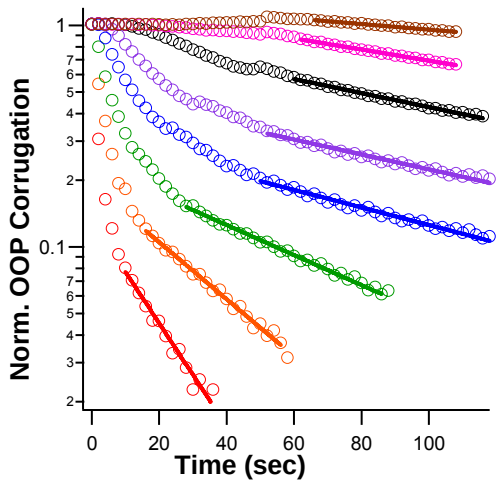






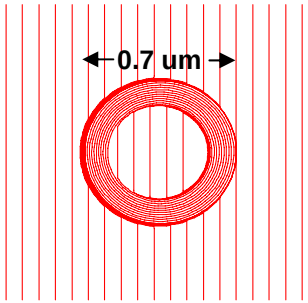






In-Plane and Out-of-Plane Corrugation Decay Time Constant Experiment vs. Simulation

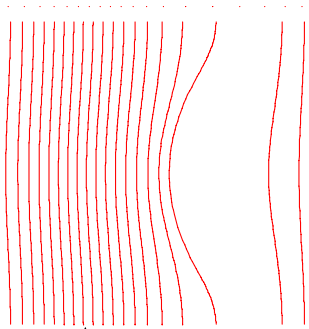
Γ=9x10^{9} A^{3}/s; $\tilde{\beta}$ = 8.35x10^{-2} meV/A; g = 1.78 meV/A^{2}



$$\frac{\tilde{\beta}}{r} > g \cdot \frac{h^3}{w^3}, \frac{h}{w} = \tan\theta \approx \theta$$

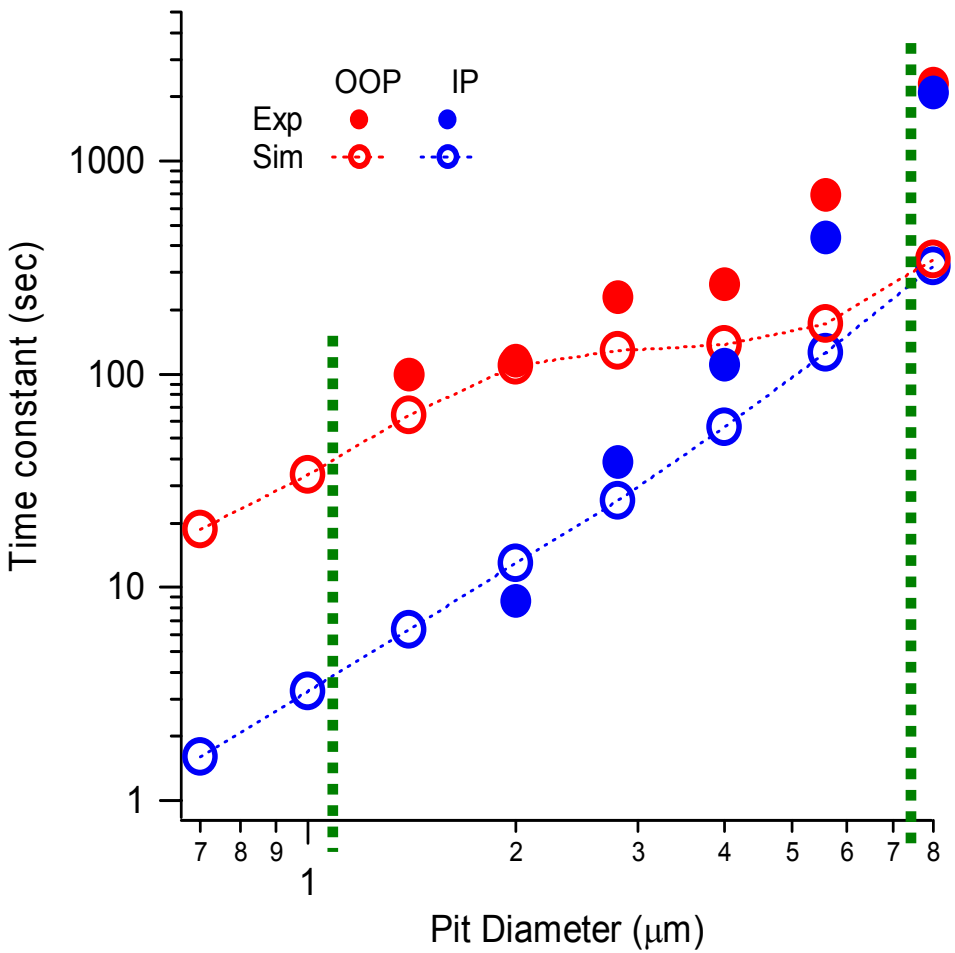
$$\frac{1}{r} \approx A \cdot \left(\frac{2\pi}{L}\right)^2, A \approx w$$

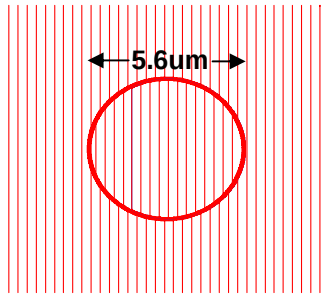
$$L < \frac{2\pi}{\theta^2} \cdot \sqrt{\frac{\tilde{\beta} \cdot h}{g}} \approx 2.2\mu m$$



$$x = A \cdot \sin\left(\frac{2\pi}{L} \cdot y\right)$$

$$\frac{1}{r} = A \cdot \left(\frac{2\pi}{L}\right)^2$$

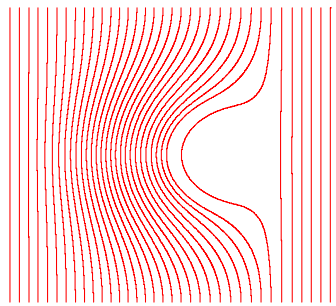




$$\frac{\tilde{\beta}}{r} < g \cdot \frac{h^3}{w^3},$$

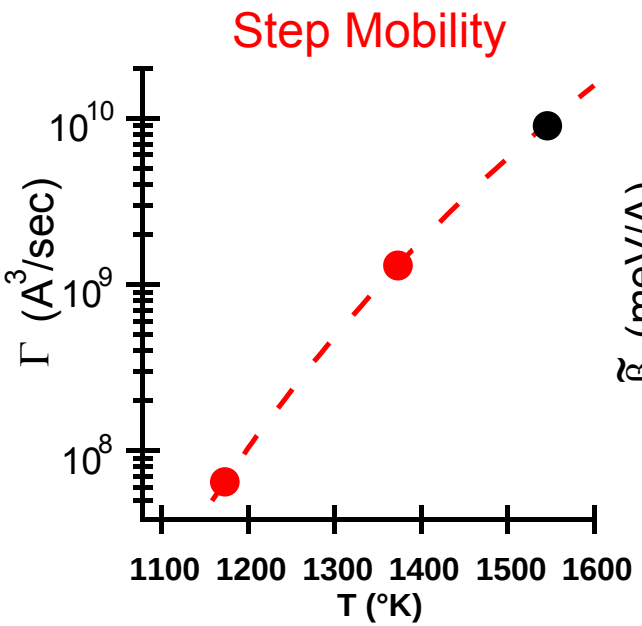
$$\frac{1}{r} \approx \langle A \rangle \cdot \left(\frac{2\pi}{L}\right)^2, \langle A \rangle \approx \frac{1}{2} \cdot \frac{d}{\sin\theta}$$

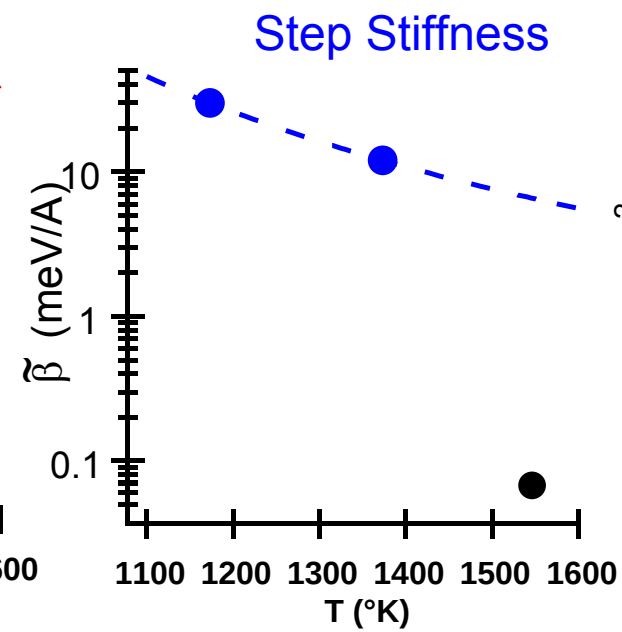
$$L > \frac{\pi}{\theta^2} \cdot \sqrt{\frac{2\tilde{\beta} \cdot d}{g}} \approx 15.5\mu m$$

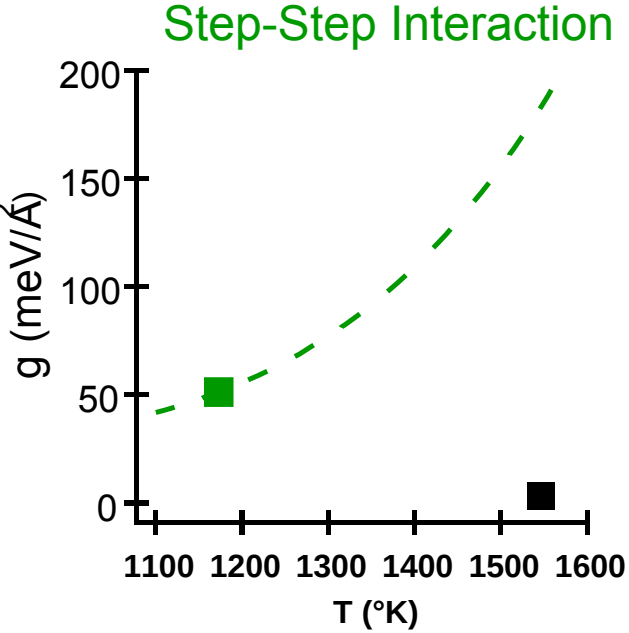


Step Kinetic Parameters for Simulation

$$\frac{d(x_n, y_n)}{dt} = \frac{\Gamma}{kT}\left(\tilde{\beta}\cdot\frac{1}{R} + gh^3\cdot\left(\frac{1}{w_1^3} - \frac{1}{w_2^3}\right)\right)\cdot\hat{n} - \left(k^+\cdot w_2 + k^-\cdot w_1\right)\cdot\hat{n}$$





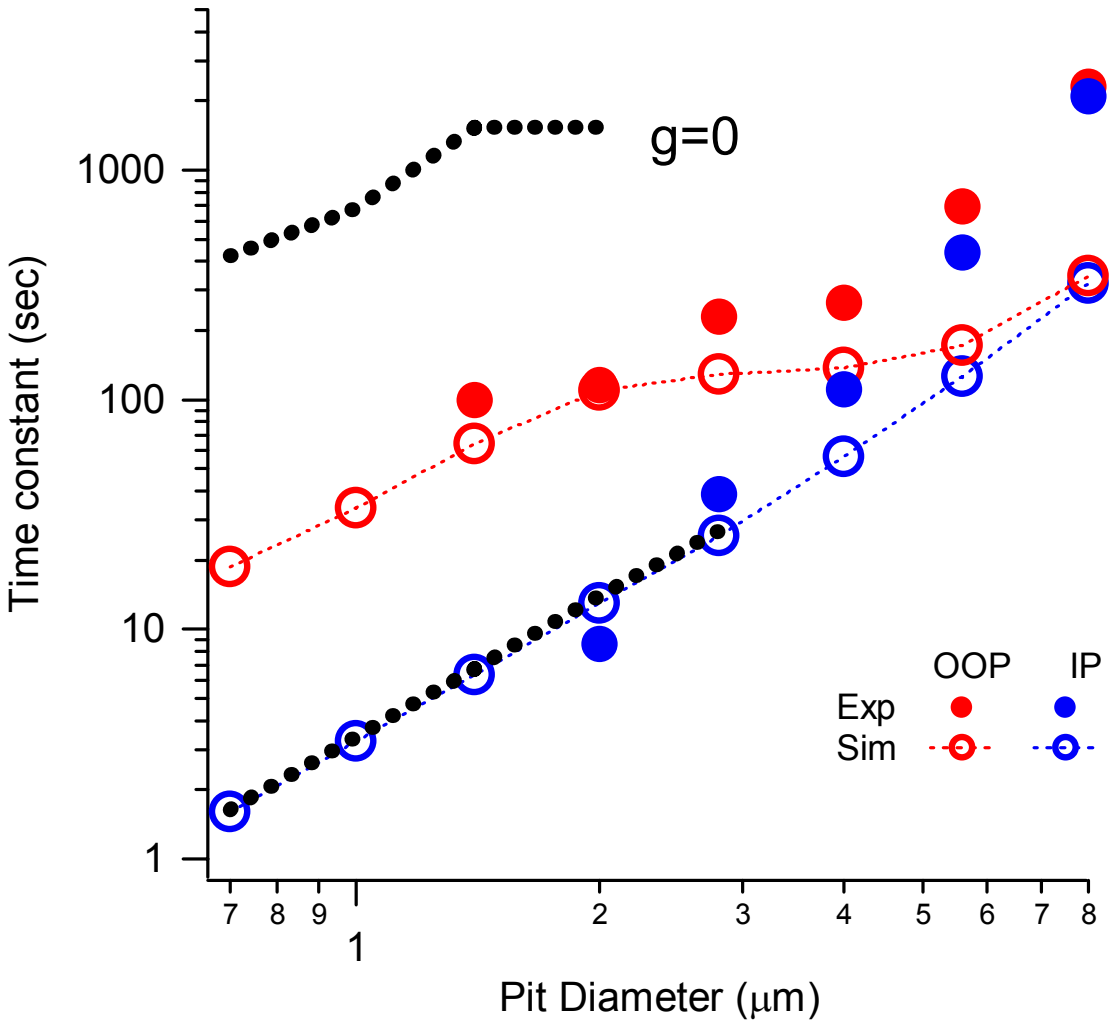


[1] N.C. Bartelt *et. al., PRB* ***48****, 15453 (1993)*
[2] S.D. Cohen *et. al., PRB* ***66****, 115310 (2002)*
[3] J.M. Bermond, *et. al. Surf. Sci.* ***416****, 430 (1998)*
[4] J.J. Metois et. al. *Surf. Sci.* ***486****, 95 (2001)*

$$g = \frac{(\pi kT)^2}{24\, h^3\, \tilde{\beta}}\left[1 + \sqrt{1 + \frac{4\, A\, \tilde{\beta}}{(kT)^2}}\right]^2$$

$k^+ = k^- =$ 1.25 BL/s * 1/2

Effect of Step-Step interaction on Corrugation Decay Time Constants



Publications

Sublimation on Patterned Vicinal Si(111)

"Characteristic Length Scales In Evolution Of Patterned Step Structure On Vicinal Si(111) Surface During High Temperature Annealing", H-C.Kan, T. Kwon and R. J. Phaneuf, in preparation (2007).

"Length-Scale Dependence of the Step Bunch Self-Organization on Patterned Vicinal Si(111) Surfaces", T. Kwon, H-C. Kan and R. J. Phaneuf, Appl. Phys. Lett. 88, 071914 (2006).

Growth on Patterned GaAs(001)

"Temperature-Driven Change in the Unstable Growth Mode on Patterned GaAs(001)", T. Tadayyon-Eslami, H.-C. Kan, L. C. Calhoun and R. J. Phaneuf, Phys. Rev. Lett. 97, 126101 (2006).

"Evolution of Patterned GaAs(001) during Homoepitaxial Growth: Size vs. Spacing," H.-C. Kan , R. Ankam, S. Shah, K.M. Micholsky, T. Tadayyon-Eslami, L. Calhoun, and R. J. Phaneuf, Phys. Rev. B 73, 195410 (2006).

"Transient evolution of surface roughness on patterned GaAs(001) during homoepitaxial growth", H.-C. Kan, S. Shah, T.T. Tadyyon-Eslami and R.J. Phaneuf, Phys. Rev. Lett., 92, 146101 (2004).