Nano Oscillator Array Intrinsic Localized Mode Pinning and Travel

Daniel Brake, Mathematics, Colorado State University, Fort Collins, CO, brake@math.colostate.edu

Vakhtang Putkaradze, Mathematics, University of Alberta, Edmonton, Canada

Ganesh Balakrishnan, Center for High Technology Materials, University of New Mexico, Albuquerque, NM

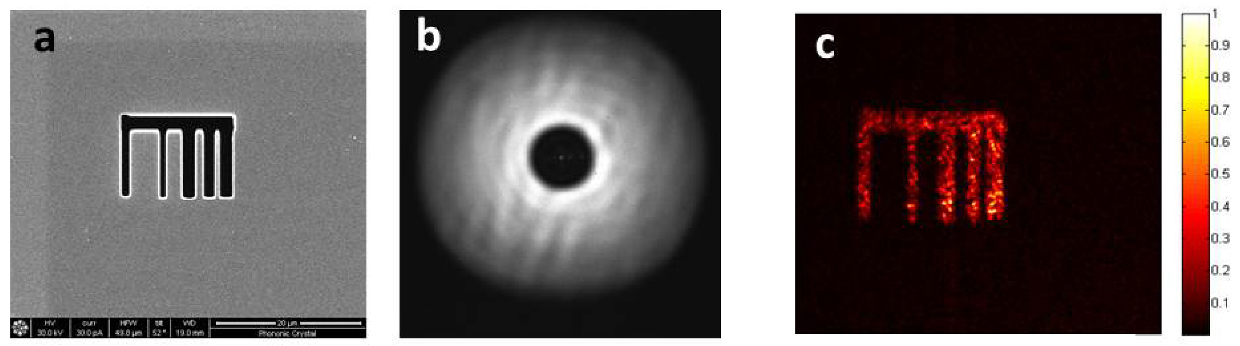
Mario Marconi, Electrical and Computer Engineering, Colorado State University, Fort Collins, CO, PI

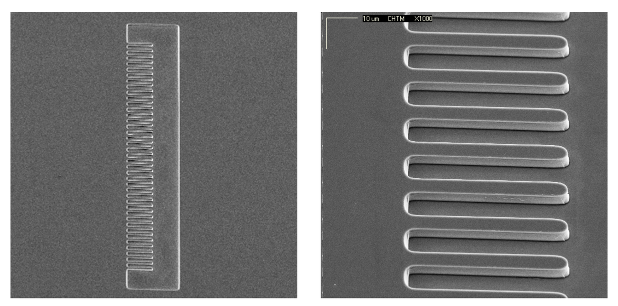
Project Overview

Single molecule detection through driven nano oscillator array

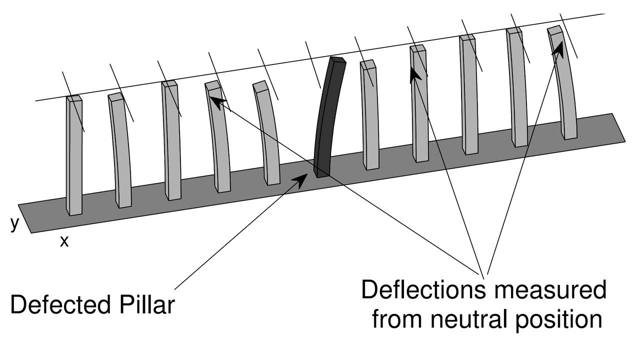
1. Monitor *amplitude* of crystal pillars; attachment of molecule to array will cause 'defect' at pillar.
2. Intrinsic Localized Mode (ILM) forms at defected location.
3. Detect change in vibration signature due to attachment defect, ⇒ molecule detection.

EUV Fourier Holography





Dry Etch & Ion Beam Crystal Manufacture



Mathematical Analysis & Modeling

Research Objectives

Modeling

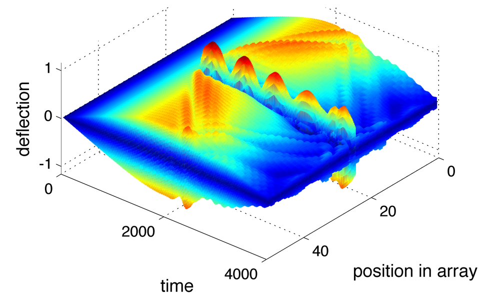
- Model *molecule attachment as ILM pinning* to defected locations in array.
- Expand previous monodirectional model [2], to be *bidirectional*.
- Simplify to low-dimensional model of ILM for quick prediction of pinning and detectability of defect *without* full simulations.
- Model *travel* of single ILM on array, similar to ILM seen in [1].
- Theoretical understanding of *ILM dynamics*.

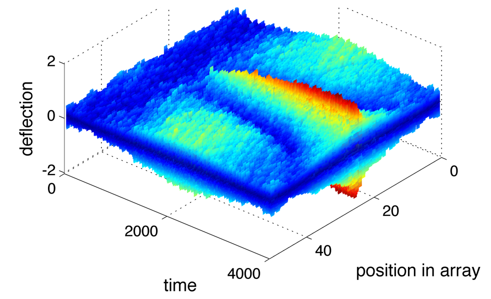
Computational Methods

Simulate both the *full bidirectional* oscillator system, and a *reduced monodirectional* system.

Full Bidirectional System [3]

- Many parameter system, derived from Hamiltonian energy. Let $u_{n,x}$ be deflection in x direction. Includes dissipation.
  - $PE = E_{2,I} + E_{2,C} + E_{4,I} + E_{4,C}$
  - $KE = \frac{1}{2}\sum_n \left(\dot{u}_{n,x}^2 + \dot{u}_{n,y}^2\right)$
  - $\mathcal{H} = PE + KE$
  - $\ddot{u}_{n,x} = -\frac{\partial \mathcal{H}}{\partial u_{n,x}}$
- Coupled system of $4n$ equations, n pillars; periodic boundary conditions.





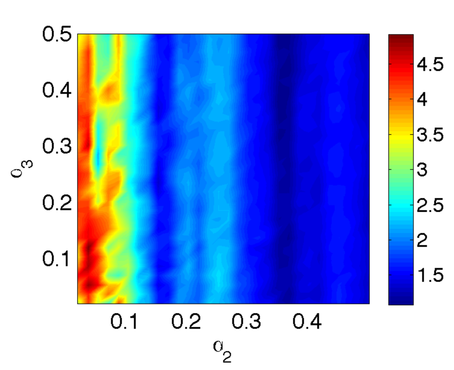
Simplified Monodirectional System [4]

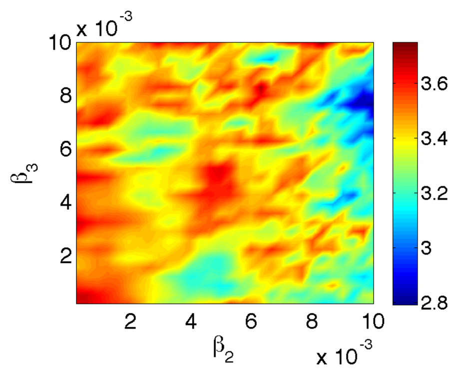
- Infinite array of nonlinear oscillators. Use Monodirectional Energy, assert symmetric exponential form of ILM, closely approximating physical ILM [2].
- Transform into canonical variables through Hamilton's equations, passing through the Lagrangian $\mathcal{L}$ and Hamiltonian $\mathcal{H}$.
- Derived *two* reduced systems:
  - Two variables: Position and velocity – x, $\dot{x}$.
  - Four variables: Position, amplitude, and their derivatives – x, $\dot{x}$, A, $\dot{A}$.
- Simulate ILM dynamics in *low-dimensional* systems with ODE solver.

Results

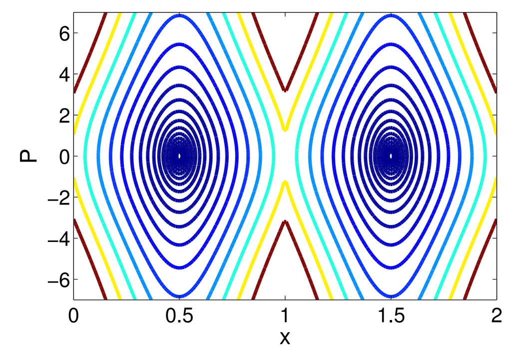
Full Bidirectional System

- **Pinning enhanced with greater defects.** Defect $>\approx$ 5% ⇒ strong detectability.
- ILM formation and pinning **immediate** from **uniform** initial condition. **Gradual** ILM formation and pinning from **random** initial conditions.
- Coupling between **directions** weakly affects ILM pinning; coupling between **adjacent pillars** much stronger.

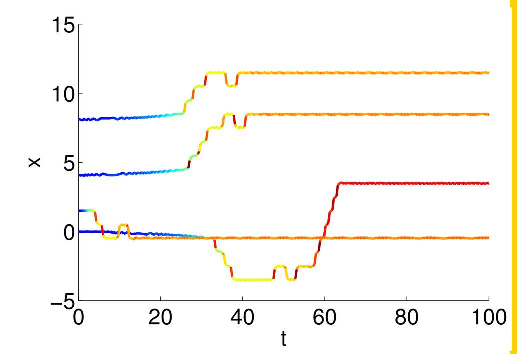




Simplified Monodirectional System



Hamiltonian level sets, with system reduced to only x.



Reduced ILM trajectories with both A and x.

- **The x-only system has simple dynamics**: periodic or escaping trajectories only, as seen from the $\mathcal{H}$ level sets on the left.
- With more realistic system, both A, x vary. We see **complex patterns of movement**, and ILM pinning happens either **at or halfway between** pillars. See right plot.

Future Research

Full system:

- Determine parameters for mis-aligned *crystalline axes.*
- Examine systems with *small inhomogeneities in all parameters*, and influence of defect on ILM formation and pinning.
- Correlate results with *physical experiments.*

Simplified System:

- Use analytic formulae to explain affect of *molecule attachment* to array.
- Make additional investigations of *complex ILM movement.*
- Expand formulae to account for *bidirectional oscillators.*
- Perform analysis for *multiple simultaneous ILM.*

Risks:

- Simplified equations may break down for *many ILMs present.*
- Mitigation: Presence of *small dissipation* in the full system *reduced appearances* of multiple ILM.

References

[1] L. Q. English, et al. "Traveling and stationary intrinsic localized modes and their spatial control in electrical lattices". *Phys. Rev. E*, 81(4):046605, Apr 2010.

[2] M. Kimura. "Studies on the Manipulation of Intrinsic Localized Modes in Coupled Cantilever Arrays". PhD thesis, Kyoto University, 2008.

[3] D. Brake, et al., "Intrinsic localized modes in two-dimensional vibrations of crystalline pillars and their application for sensing". *Japanese Journal of Applied Physics, under consideration*, 2012.

[4] D. Brake, V. Putkaradze, "Simplified models for Intrinsic Localized Mode dynamics". *NonLinear Theory and Applications, accepted*, 2012.

Acknowledgements

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