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

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.
- $PE = E_{2,1} + E_{2,3} + E_{4,1} + E_{4,3}$
- $KE = \frac{1}{2} \sum_n (\ddot{u}_{n,x} + \ddot{u}_{n,y})$
- $H = PE + KE$
- $\ddot{u}_{n,x} = -\frac{\partial}{\partial u_{n,x}} H$
- Coupled system of $4n$ equations, $n$ pillars; periodic boundary conditions.

Simplified Monodirectional System [4]
- Transform into canonical variables through Hamilton’s equations, passing through the Lagrangian $L$ and Hamiltonian $H$.
- 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 $\geq 5\% \Rightarrow$ 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
- The $x$-only system has simple dynamics: periodic or escaping trajectories only, as seen from the $H$ level sets on the left.
- With more realistic system, both $A, \dot{A}$ 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


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