

ILM Formation in Arrays of Nonlinearly Coupled Bidirectional Crystal Oscillators

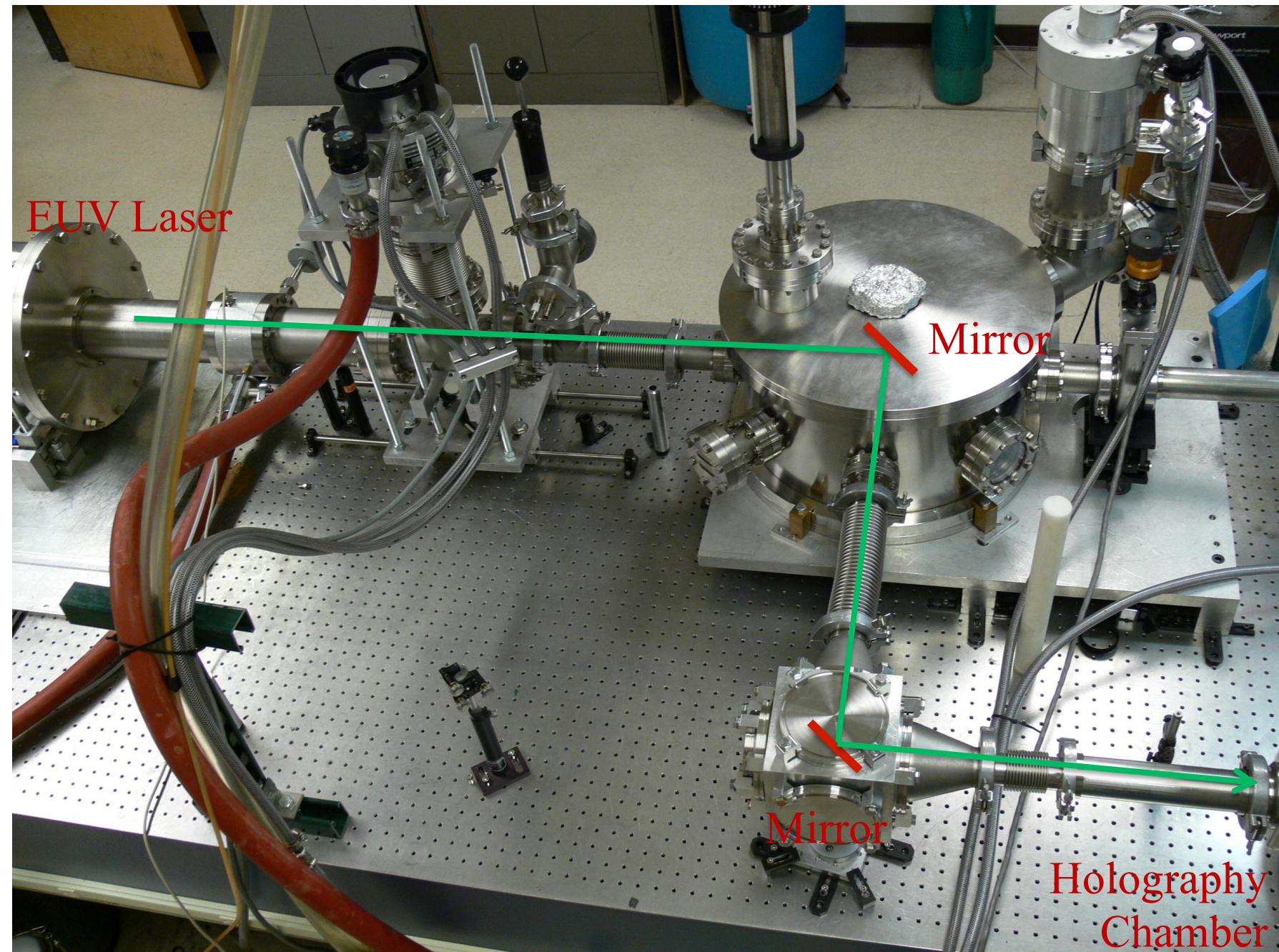
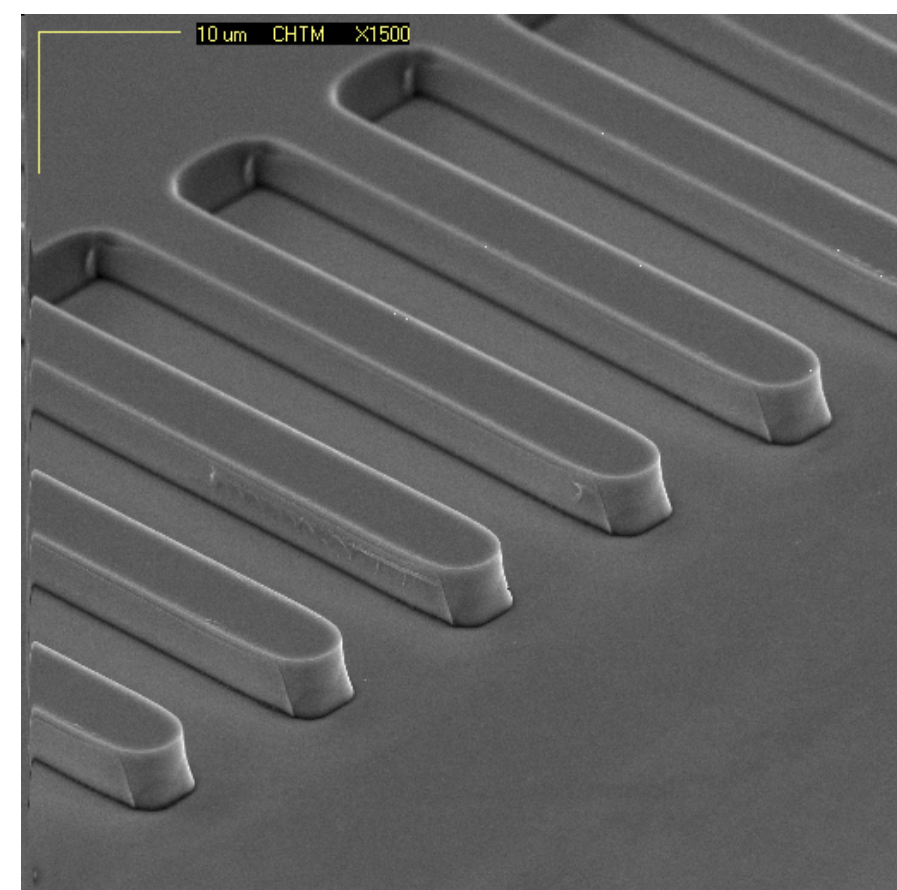


D. Brake², M. Marconi¹, V. Putkaradze², G. Balakrishnan³
NSF Engineering Research Center for Extreme Ultraviolet Science & Technology and
¹Department of Electrical and Computer Engineering, Colorado State University
²Department of Mathematics, Colorado State University
³Department of Electrical and Computer Engineering, University of New Mexico

Motivation and Goals

Single molecule detection using a single vibrating crystal pillar has been implemented previously, by monitoring the shift in frequency of the pillar upon attachment of the contaminant. The frequency of this vibration is extremely high for nano-scale crystals, so a very fast light source is necessary.

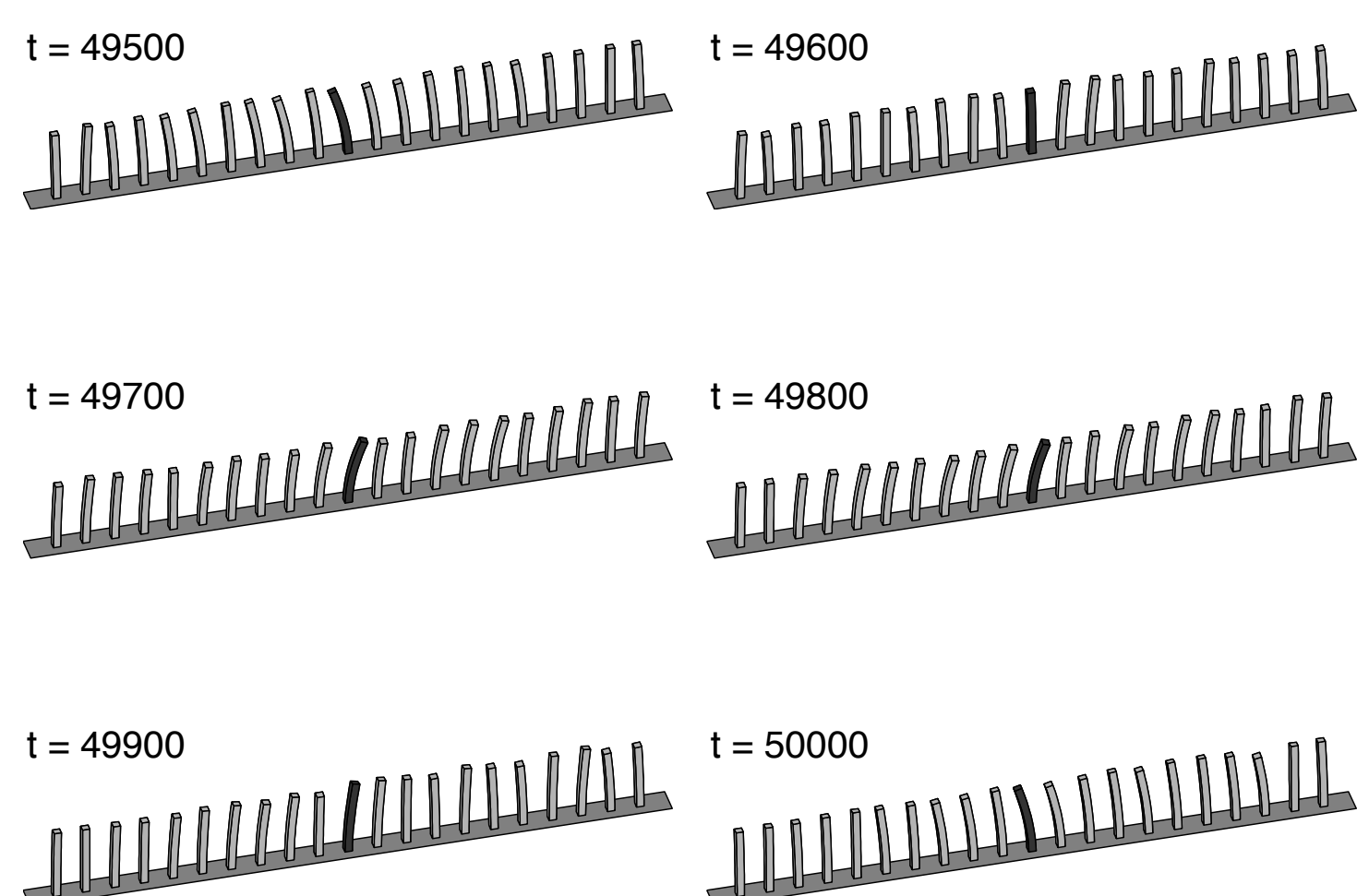
Using an array of crystals rather than a single oscillator, we can monitor the amplitude envelope rather than the frequency shift. By deliberately placing defects into the array with regular spacing, special wave forms called Intrinsic Localized Modes (ILMs) form, and become pinned at the defects. When a molecule attaches to a pillar in the array, the shape of the entire envelope will change, and using Fourier Transform Holography, we can detect the change.



Intrinsic Localized Modes

ILM is a special oscillatory mode which spontaneously develops in an array of oscillators in which a defect is present. The defect may be due to a manufacturing error, could be deliberate, or could be temporary due to attachment of a particle.

The form of an ILM is such that the energy of the vibration becomes concentrated at the defect. Further, the entire form of the vibration changes upon defect, not merely the amplitude at the defect. This makes it possible for us to monitor ILM envelopes, to detect single molecule attachment to a nanosensor array.



Graphical depiction of bidirectional ILM in crystal array. Defect at dark pillar, the amplitude of vibration becomes concentrated at defect.

Simulations

A Hamiltonian for the system of oscillators gives rise to the equations of motion. Our energy functional is:

$$E = E_2 + E_3 + E_4$$

The energy is the sum of quadratic terms, which give rise to the linear terms in the equations of motion, and higher order terms. The orientation of the crystalline axes to the pillar faces determine the form of the H.O.T. For now, we assume the faces to be in line with the principle axes of the crystal structure, so the cubic terms E_3 in E are assumed to be 0. We take only quartic terms.

$$E_2 = \frac{1}{2} \sum_k \alpha_{1,x} u_{k,x}^2 + \alpha_{1,y} u_{k,y}^2 + \alpha_{2,x} (u_{k,x} - u_{k-1,x})^2 + \alpha_{2,y} (u_{k,y} - u_{k-1,y})^2 + \alpha_{3,y} (u_{k,x} - u_{k,y})^2$$

$$E_4 = \frac{1}{4} \sum_k \beta_{1,x} u_{k,x}^4 + \beta_{1,y} u_{k,y}^4 + \beta_{2,x} (u_{k,x} - u_{k-1,x})^4 + \beta_{2,y} (u_{k,y} - u_{k-1,y})^4 + \beta_{3,x} (u_{k,x} - u_{k,y})^4$$

We formulate the equations of motion by taking the derivative of the energy with respect to the deflection variable u for the n th pillar, in both the x - and y -directions. Presented here are only the x equations. Using Runge-Kutta 45 ODE solver, we evolve random initial conditions forward in time.

$$\ddot{u}_{x,n} = -\frac{\partial E}{\partial u_{x,n}} \quad \ddot{u}_{y,n} = -\frac{\partial E}{\partial u_{y,n}}$$

$$\ddot{u}_{x,n} = -\{\text{linear} + \text{nonlinear}\} + \sigma \sin(t) - \gamma \dot{u}_{x,n}$$

$$\text{linear terms} = \alpha_{1,x} u_{x,n} + \alpha_{2,x} ((u_{x,n} - u_{x,n-1}) + (u_{x,n} - u_{x,n+1})) + \alpha_{3,x} (u_{x,n} - u_{y,n})$$

$$\text{nonlinear terms} = \beta_{1,x} u_{x,n}^3 + \beta_{2,x} ((u_{x,n} - u_{x,n-1})^3 + (u_{x,n} - u_{x,n+1})^3) + \beta_{3,x} (u_{x,n} - u_{y,n})^3$$

The parameters in the system are:

- α_1 : linear restoration coefficients
- α_2 : linear coupling for adjacent members of the array
- α_3 : linear coupling for bidirectional vibration
- σ : amplitude of driving
- γ : damping coefficient
- β_1 : cubic restoration coefficients
- β_2 : cubic coupling for adjacent members of the array
- β_3 : cubic coupling for bidirectional vibration

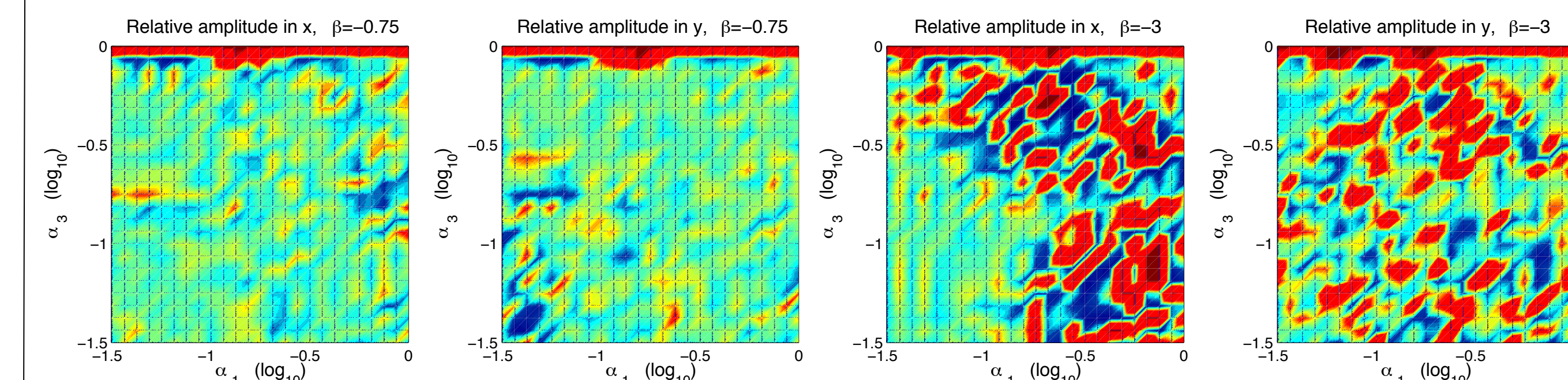
- Note that each of the α and β parameters can have different values in x and y directions.

Future Work

- Perform comprehensive parameter sensitivity study.
- Determine threshold forcing amplitude for blowup of array
- Work with experimentalists to determine actual values of parameters.
- Use homotopy continuation to find and characterize all ILM's for system with cubic Hamiltonian.

Results

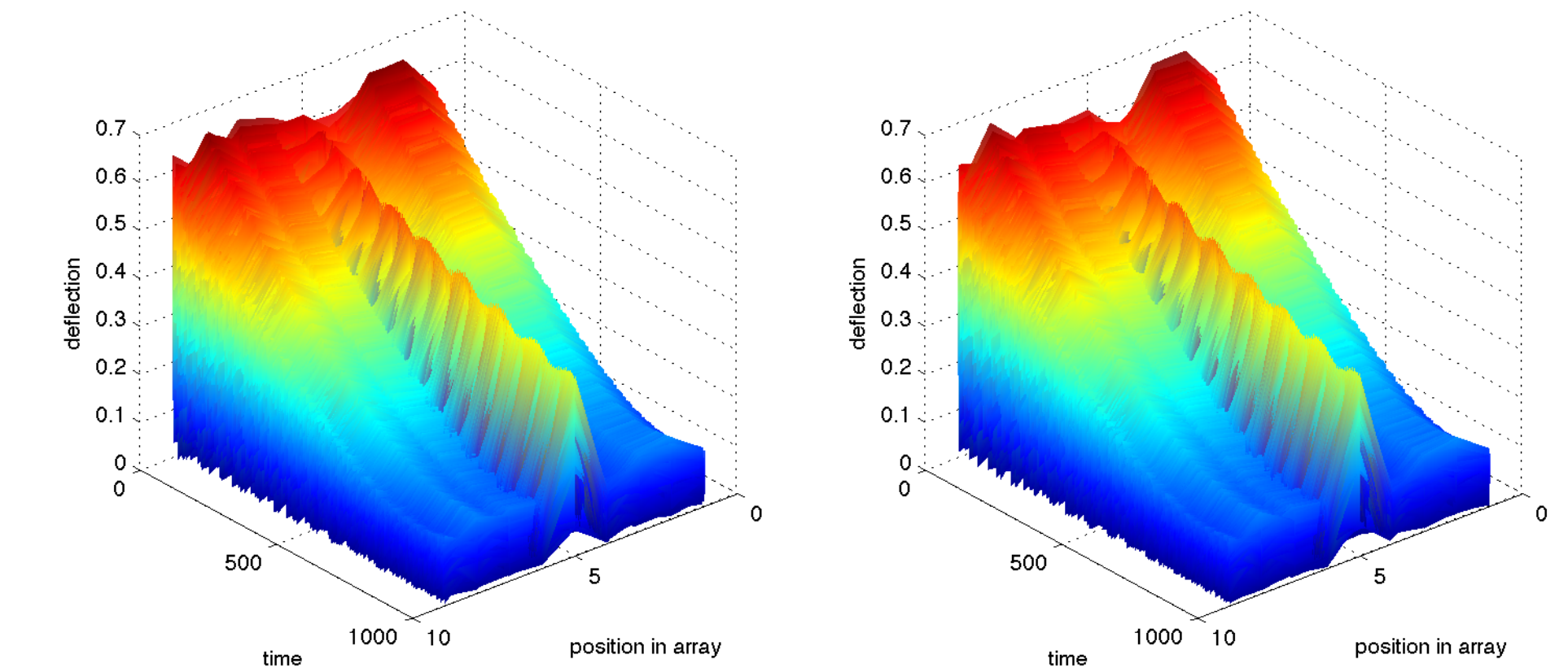
Precise and reliable modeling of the sensor array dynamics is important, because the phase map, in terms of parameters in the system, is so complicated. Some regions indicate the presence of ILM, whereas other do not.



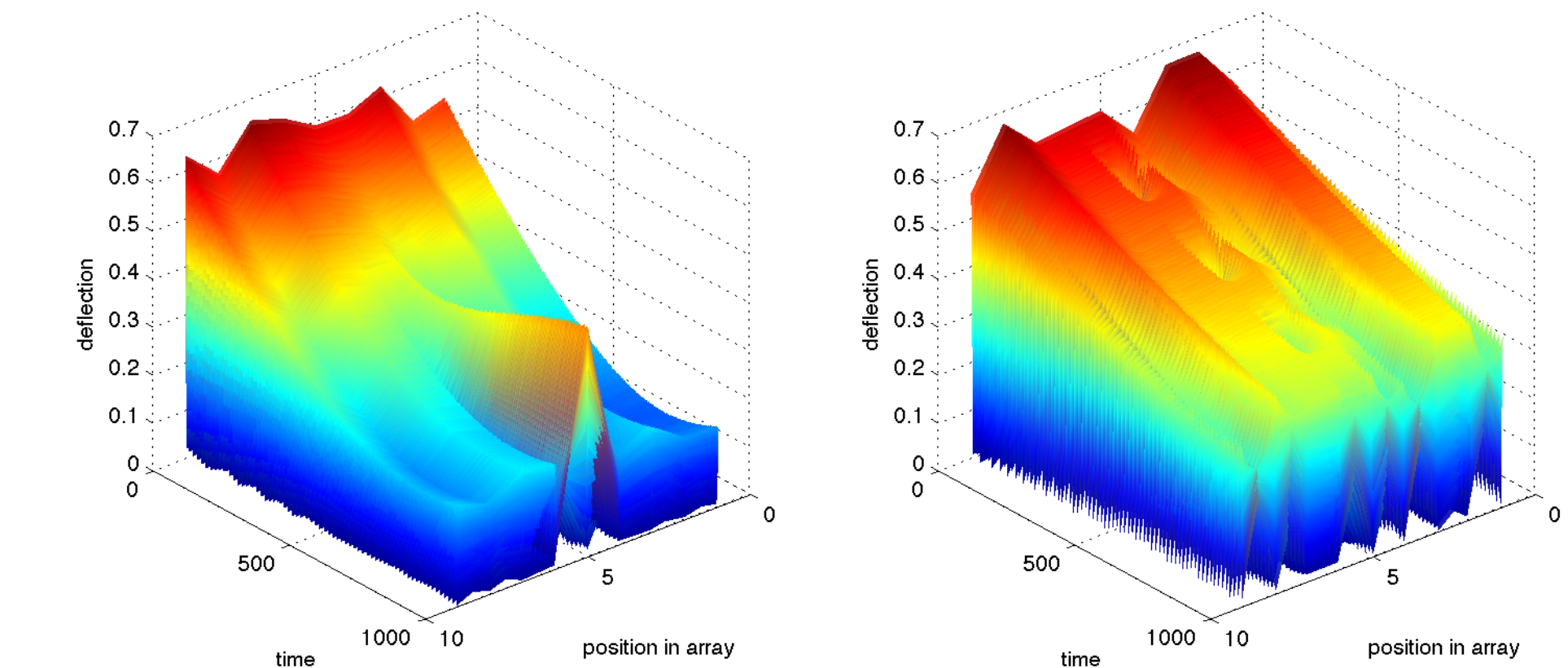
Above Left: For $\beta_3 = 10^{-0.75}$, have strong ILM presence in both vibration directions near $\alpha_3 = 1.0$, but weak presence elsewhere.

Above Right: For $\beta_3 = 10^{-0.75}$, have strong ILM presence in same region. However, the rest of phase space has islands of ILM's, with formation in both directions occurring only sometimes.

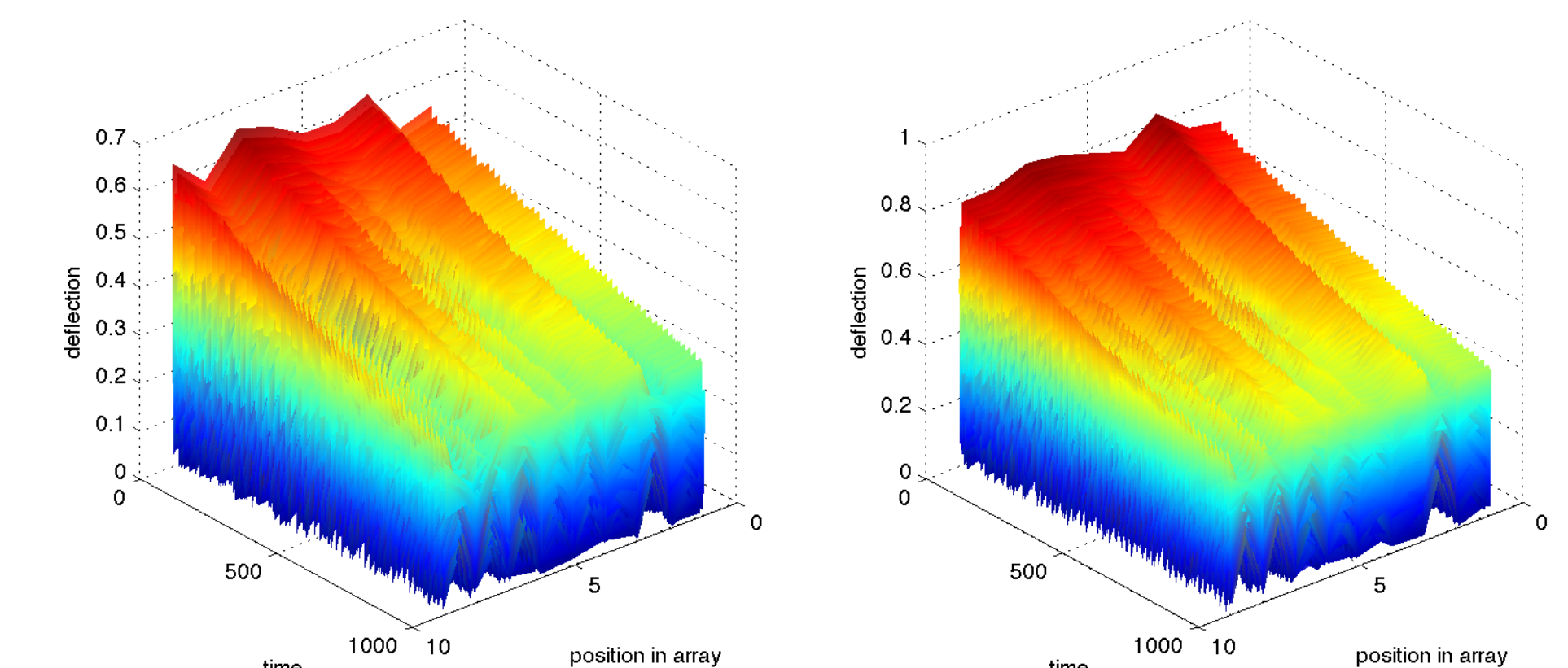
Below: Examples of ILM formations.



An ILM forms in both the x - and y -directions of vibration.



An ILM forms only in the x -direction, while y -direction remains random..



An ILM forms in *neither* direction of vibration.

Acknowledgements

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