# Intrinsic localized modes in two-dimensional vibrations of crystalline pillars

Daniel Brake[†] and Vakhtang Putkaradze[†,‡]

[†] Department of Mathematics, [‡] School of Biomedical Engineering
Colorado State University, Fort Collins CO 80523
Email: brake,putkarad@math.colostate.edu

**Abstract**—We study the appearance of ILMs in a model for the two-dimensional vibrations of an array consisting of mono-crystal nanopillars. For these pillars, the elastic properties and hence the dynamics depend on the pillar's shape and the orientation of the crystal axes. We show that ILMs do form in the system, but their stability, defect pinning and reaction to friction strongly depend on the crystals properties, with the optimal dynamics only achieved in a rather small region of the parameter space.

## 1. Introduction

The existence of the Intrinsic Localized Modes, or ILMs, has been demonstrated in many coupled systems of oscillators. These coherent oscillations were first discovered in [1, 2]. ILMs have then been found in a wide variety of structures, and there has been substantial interest in the theoretical analysis and practical applications of these structures [3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]. In general, most of these works have concentrated on the analysis of the oscillations being described by one variable that is perhaps allowed to be complex. In particular case of ILM in cantilever arrays, the one-dimensionality of vibrations was enforced by designing the experiments with the cantilever thickness in the direction of vibration to be much smaller than in the other direction. However, modern application of ILMs to areas like sensing require miniaturization of the nanopillar arrays to sub-micron levels [15]. Cantilever arrays of this size are fabricated using techniques like nanoheteropitaxy [16], typically producing pillars with similar transversal sizes, which thus do not typically possess a preferred direction for vibration. Driving these cantilever arrays at their resonant frequencies typically excites vibration modes with deflection in both directions. The goal of this paper is to analyze the appearance of ILMs in the case when oscillations in both directions are allowed. The two-dimensional motion of the pillars is similar to having two coupled oscillator arrays, or an array of oscillators with an internal degree of freedom. While there has been considerable amount of work in this area already, see for example [17, 18, 19], the difference between our work and previous studies is in the structure of elastic coupling between two directions of oscillation.

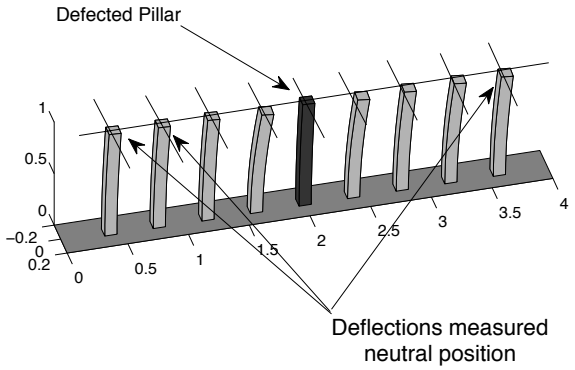


Figure 1: A cartoon of one dimensional cantilever array that is able to undergo vibrations in two directions. For illustration, we have also drawn a defected pillar that is used to pin the ILM appearing from random initial condition on the center pillar.

## 2. Setup of the Problem

For simplicity, in this paper we assume that each crystalline pillar in the array has a square cross-section, with the flat sides being parallel to the axis of the crystal, and the pillar material is such that crystalline axes are parallel to the pillars' sides and perpendicular to each other. These cantilever arrays, when driven by an external vibration source, function as coupled oscillators. The material properties determine the governing differential equations, which are a generalization of the nonlinear equations for pillar vibrations derived earlier. In order to reliably pin the ILM to the desirable location (center pillar), we introduce a small defect in that pillar's properties, and make sure that the ILM is attractive to the defect. The setup for the problem of interest is shown on Fig. 1. In an experiment with sub-micron nanopillar arrays, the forcing will most likely be distributed among many pillars and artificial preparation of an ILM will be experimentally unfeasible. Thus, in all our simulations, we have analyzed ILMs that spontaneously and robustly appear from random initial conditions, under the influence of distributed forcing.

The equations of motion for the pillars are formulated

as follows. Let $u_k$ be the deflection of the $k$-th crystal pillar from its neutral position. A typical equation, describing the evolution of one dimensional deflection in a one-dimensional array is given by the equation

$$\begin{aligned}\ddot{u_k} = &-\alpha_1 u_k - \alpha_2((u_k - u_{k-1}) + (u_k - u_{k+1})) \\ &- \beta_1 u_k^3 - \beta_2((u_k - u_{k-1})^3 + (u_k - u_{k+1})^3) \end{aligned} \quad (1)$$

Here, $\alpha_1, \alpha_2, \beta_1, \beta_2$ are the constants that are determined by the material properties of the pillars as well as the geometry. In order to describe the two-dimensional deflection of the pillars, we introduce two components of the pillar deflection as $\mathbf{u}_k = (u_{k,x}, u_{k,y})$ that are not necessarily aligned with the crystal axes. The linear components of the stress can be computed as follows. Suppose for the given deflection, the linear part of deformation energy is given by the quadratic form $E_2 = \frac{1}{2}\mathbf{u}_k^T Q_2 \mathbf{u}_k$. For the purpose of this paper, we choose a parameterization of the symmetric matrix $Q_2$ with three parameters $\alpha_{1,x}$, $\alpha_{1,y}$ and $\alpha_3$ as follows:

$$E_2 = \frac{1}{2}\sum_k \alpha_{1,x} u_{k,x}^2 + \alpha_{1,y} u_{k,y}^2 + \alpha_3 (u_{k,x} - u_{k,y})^2 . \quad (2)$$

For the purposes of simplified analysis in this paper, we only consider $\alpha_{1,x} = \alpha_{1,y} = \alpha_1$ which we treat as a parameter. Then, we study the behavior of the system as a function of parameters $\alpha_1$ and $\alpha_3$. Note that this is somewhat different from the standard normalization, where one of the natural frequencies would be normalized to 1. Also, it is important to notice that the eigenvalues of the Hessian of this matrix are strictly positive and distinct for $\alpha_1 > 0$ and $\alpha_3 > 0$ so there are no degeneracies or unphysical values of parameters in the system.

The nonlinear (cubic) term in the equation leads to the fourth order term in energy, described by a fourth order tensor $Q_4$, *i.e.*, $E_4 = Q_4 \cdot \mathbf{u}_k \cdot \mathbf{u}_k \cdot \mathbf{u}_k \cdot \mathbf{u}_k$. Even when proper symmetries are included, the number of non-zero components of $Q$ lead to the exceedingly large number of parameters. It is possible to estimate some of these components analytically if the information about the orientation of crystalline axes, pillar shape and nonlinear elasticity is known. This will be done in further studies; for the purpose of this work, we shall consider a simpler particular case of the nonlinear coupling energy as

$$E_4 = \frac{1}{4}\sum_k \beta_2\left(u_{k,x}^4 - u_{k,y}^4\right) + \beta_3\left(u_{k,x} - u_{k,y}\right)^4 . \quad (3)$$

The total potential energy is then $E = E_2 + E_4$. For symmetry reasons, in the case considered here there is no cubic term in the energy. However, note that a cubic term may appear for a general arrangement of the crystal axes and pillar facets, in the geometries breaking the reflection symmetry of the system. The appearance and role of a cubic term in energy, leading to quadratic terms in the equations, is very interesting and will be addressed in further studies. This will lead to the necessity of investigation of a large number of parameters, which we are not going to do here. The corresponding equations of motion for two directions are

$$\begin{aligned}\ddot{u_{k,x}} = &-\alpha_{1,x} u_{k,x} - \alpha_2((u_{k,x} - u_{k-1,x}) + (u_{k,x} - u_{k+1,x})) \\ &- \beta_1 u_{k,x}^3 - \beta_2((u_{k,x} - u_{k-1,x})^3 + (u_{k,x} - u_{k+1,x})^3) \\ &- \alpha_3(u_{k,x} - u_{k,y}) - \beta_3(u_{k,x} - u_{k,y})^3 \\ &- \gamma \dot{u}_{k,x} + \sigma \sin(t) \end{aligned} \quad (4)$$

$$\begin{aligned}\ddot{u_{k,y}} = &-\alpha_{1,y} u_{k,y} - \alpha_2((u_{k,y} - u_{k-1,y}) + (u_{k,y} - u_{k+1,y})) \\ &- \beta_1 u_{k,y}^3 - \beta_2((u_{k,y} - u_{k-1,y})^3 + (u_{k,y} - u_{k+1,y})^3) \\ &- \alpha_3(u_{k,y} - u_{k,x}) - \beta_3(u_{k,y} - u_{k,x})^3 \\ &- \gamma \dot{u}_{k,y} + \sigma \sin(t) \end{aligned} \quad (5)$$

This functional form of directional coupling allows a comprehensive study of ILM formation for two parameters, $\alpha_3$ and $\beta_3$. In addition, we have added the dissipation in the pillars, described by the term $\gamma\dot{\mathbf{u}}_k$, and the forcing term, proportional to $\sigma$. The coupling parameters $\alpha_3$ and $\beta_3$ can be estimated numerically, but their precise value for a given experiment is generally unknown. Thus, they must be treated as parameters in the problem.

## 3. Results

Here, we present the results for spontaneous formation of ILMs in the system. The values of other parameters are presented in the table below. For completeness, we present the values of the other parameters used in simulations below. While the typical value of $\alpha_1$ are around 1, we have chosen to scan a large set of values in order to accommodate both cases when there is large discrepancy in natural frequencies in two directions, and, alternatively, when the natural frequencies of vibration are very close to each other.

| Parameter | Value |
|---|---|
| $\alpha_1$ | $0.0001 \ldots 1$ |
| $\alpha_3$ | $0.0001 \ldots 1$ |
| $\beta_1$ | 0.01 |
| $\beta_2$ | 0.0001 |
| $\beta_3$ | 0, 0.001 |
| $\gamma$ | 0.001 |
| $\sigma$ | 0.01 |

The results of our simulations are presented on Fig. 2 and Fig. 3. We plot the ILM detectability, *i.e.*, the energy concentrated in an ILM divided by the average energy of a pillar, which is non-zero due to the competition between the forcing and dissipation. Each point on this plot is the result of simulation until $t = 300$, with the amplitude of ILM computed from the last half of the time interval. The horizontal and vertical axes are $\alpha_3$ and $\alpha_1$, respectively. Red areas represent high values of detectability, and blue represent the low values. As we see, there are areas of parameter where ILM appearance is very robust; however, these areas

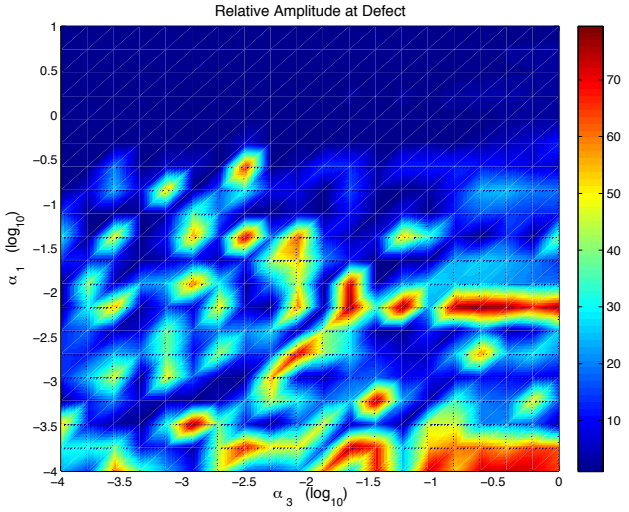


Figure 2: Phase diagram for ILM presence in 9-pillar crystal array. Coupling parameters $\alpha_1$ and $\alpha_3$ are examined for $\beta_3 = 0$. Red denotes strong ILM formation whereas blue indicates practically no spontaneously forming ILMs present in the system. In order to scan large areas of parameters we use logarithmic scale for $\alpha_1$ and $\alpha_3$.

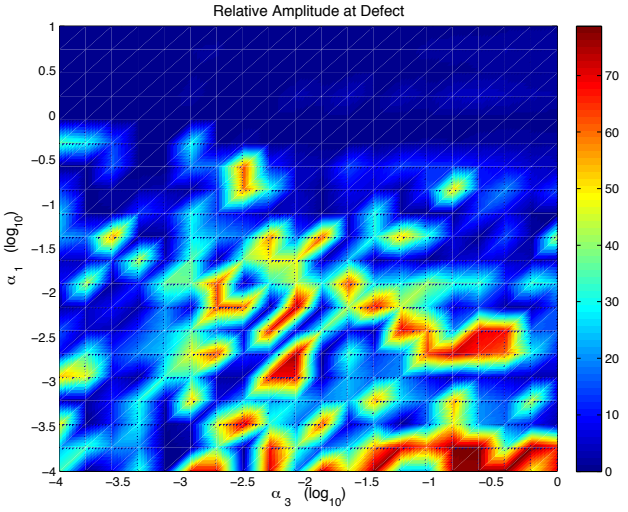


Figure 3: Same phase diagram as in Figure 2 but computed for $\beta_3 = 0.001$

are relatively small. There is a highly intricate pattern describing high detectability of ILMs, and it is more typical to observe the energy concentration in ILM to be rather small, as is evident from our results. Thus, the preliminary work presented here warrants more detailed studies of ILM formation and detectability, and the necessity of improved design of nanopillar arrays for nanotechnology applications.


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