# Numerical Simulation of Nonlinear Vibration Modes in a Small Number Atomic System

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**Abstract**—In this study, we investigate nonlinear vibration modes of an atomic system which consists of six particles. The nonlinear vibration modes are continued from phonon modes of the system. Relation between frequencies and amplitude are discussed. Linear stability of the nonlinear vibration modes is also analyzed. It is found that, in some range of initial amplitude, energy exchange is observed between a few vibration modes.

## 1. Introduction

Nonlinearity of interaction potential between atoms in crystals plays an important role in dynamics in large displacement of atoms such as structural change which is realized by overcoming the potential barriers between two stable states. However, it is well known that nonlinear dynamics such as instability and energy transfer between phonon modes are complex and has not been clarified. In this study, we focus on nonlinear normal modes which is continued from normal modes in small amplitude limit. We investigate structure and stability of the nonlinear normal modes for well understanding of nonlinear dynamics of atomic vibration.

## 2. Model

We consider atomic cluster which consists of 6 atoms. Hamiltonian of the system is given by

$$\frac{H}{\varepsilon} = \frac{1}{2}\sum_{i=1}^{6} \dot{\boldsymbol{q}}_i \cdot \dot{\boldsymbol{q}}_i + \sum_{i=1}^{6}\sum_{\substack{j=1\\ j\neq i}}^{6} \phi(d_{ij}), \quad (1)$$

where $\dot{\mathbf{q}}_i$ is a velocity of $i$-th atom, $d_{ij} = \left|\mathbf{q}_j - \mathbf{q}_i\right|$ is distance between $i$-th and $j$-th atoms. Interaction $\phi(d)$ between two atoms given by Morse potential,

$$\phi(d) = \varepsilon[e^{-2A(d-d_0)} - 2e^{-A(d-d_0)}], \quad (2)$$

where $\varepsilon = 1.0$, $A = 1.0$ and $d_0 = 6.0$.

It is known that there are two stable structures on considering condition: OCT (Octahedron) and CTBP (Capped trigonal bipyramid) [1–4].

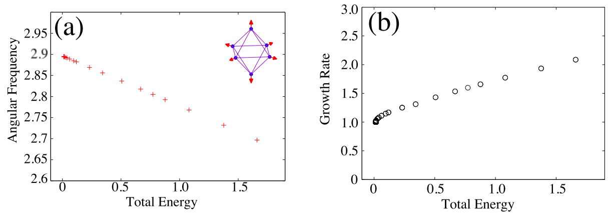


Figure 1: Relation between (a)frequency and energy, and (b) maximum growth rate and energy.

## 3. Results and Discussion

Numerical solutions of the nonlinear normal modes of OCT are searched form the normal modes by shooting method. Fig.1(a) shows that the relation between energy and frequency of an obtained nonlinear normal modes. Due to the soft nonlinearity of Morse potential, the frequency decreases as the energy decreases.

Linear stability is also investigated numerically. Fig.1(b) shows the maximum growth rates of perturbations around the nonlinear normal modes. It is found that the critical energy of instability exists.

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## References

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