Nonlinear Energy Localization Modes in Crystals: Discrete Breather

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ABSTRACT

Nonlinear vibration modes called discrete breathers (DBs) in crystals are investigated by molecular dynamic simulations. Numerically precise solutions of the DB in two dimensional graphene are calculated and its properties are investigated. It is found that the calculated DB reflects nonlinearity of interactions between atoms. Moreover linear stability analysis of the DB under uniaxial strain is performed. Complex behavior of growth rate has observed depending on the strain as well as the period of the DB. Displacement of the some unstable modes localized around the DB. This result shows the possibility that the DB can be a starting point of change of the structure of crystals.

Key words: Energy Localization, Discrete Breather, Molecular Dynamics

1. INTRODUCTION

Vibrational property is one of the most fundamental dynamical properties of crystal. Phonon dispersion relation reflects not only the structure of crystals but also macroscopic properties of solid such as elastic constants. It should be emphasized that theories of vibration are based on the lattice dynamics of theoretical lattices that is investigated in mathematical physics. From these points of view, it can be said that the material science and the mathematical physics can be related closely. When we consider problems of vibration, small amplitude limit is often considered. In this case, we deal with the linear equations of motion. Linearization makes the problem much easier without losing some important characteristics. However if we interested in problems in that the linear approximation is invalid, nonlinear dynamics should be considered. It has been known that nonlinearity of the system reproduce richer dynamics such as instability, bifurcation and pattern formation. Recently, energy localization called discrete breathers (DB) or intrinsic localized modes (ILM) [1] has been extensively studied in physics and mathematics [2]. DB is characterized as (i)vibration modes that have frequency out of the linear phonon band, (ii)large amplitude vibrations with small numbers of atoms, and (iii)vibration modes that exist wade class of the system, that is, the DB can be excited in any dimension of the system, without requiring any integrability of the system. Therefore it is expected that the DB appears in various physical phenomena. Indeed, it has been reported that DB is observed in various physical systems such as micromechanical cantilever array [3], macroscopic mechanical structures [4], and waveguide array [5]. Crystal structure is one of the most desirable physical systems that the DB is excited in atomic scales. In this study, we show some numerical results that appearance of DB in two dimensional atomic structures by molecular dynamics simulations.

2. MODELS

We show the some results of two dimensional dynamics of carbon atoms in graphene. Figure 1 shows the models of our simulation. Carbon atoms form two-dimensional sheet with honeycomb structure. Total number of atoms in the system is 180. Periodic boundary conditions are considered in x-direction, and fixed boundary condition is considered in y-direction, respectively. We investigate the dynamics of atoms by molecular dynamics method. Interaction between carbon atoms is described by the Brenner potential [6]. Equilibrium length between neighboring atoms is 0.145nm. Note that we perform simulation without any heat bath. We use the velocity Verlet method for numerical integration of the equations of motion. Time step for the numerical integration is 0.01fs.

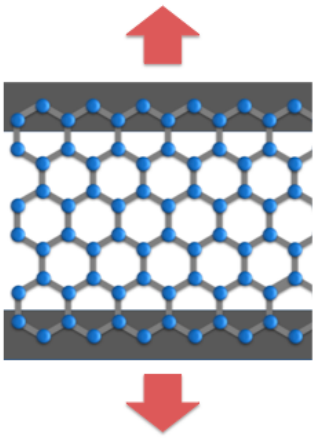


Fig1. Model

3. RESULTS AND DISCUSSION

At first, we search precise numerical solutions of DBs in graphene. Numerical method is described in [7] in detail. Figure 2 shows snapshots of the DB that is excited in graphene. Two neighboring atoms in center vibrate with large energy. However surrounding atoms are almost rest. In small amplitude vibration, it is expected that energy of vibration spread out to the surrounding atoms. In our case, however, the vibration mode is confined to narrow region and energy does not spread out to the surrounding atoms. This fact is also confirmed by Fig.3. Figure 3 shows the temporal evolution of displacement of two atoms at which DB is excited. As long as the period of the numerical simulation, atoms vibrate stably. Figure 4 shows the relation between the amplitude and frequency of DB. It is found that the frequency of DB depends on its amplitude. This is quite different from those in the linear phonon mode, which does not depend on the amplitude of the vibration. Therefore the observed DB is highly affected by nonlinearity of the interaction between atoms.

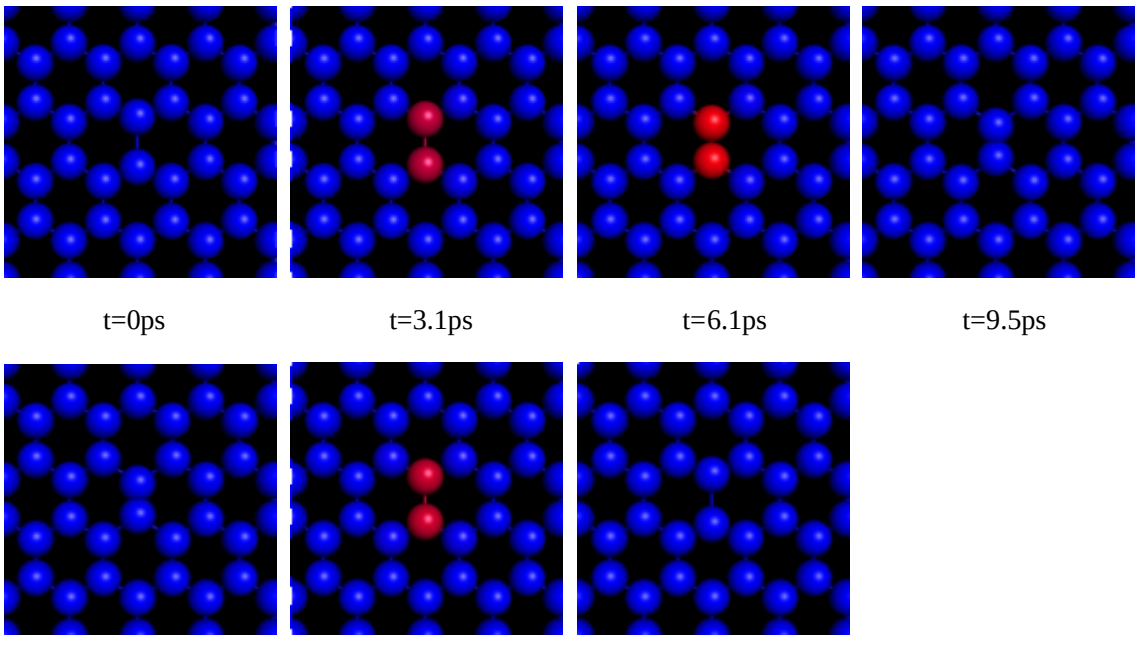


Fig.2 Snapshot of vibration of DB in graphene

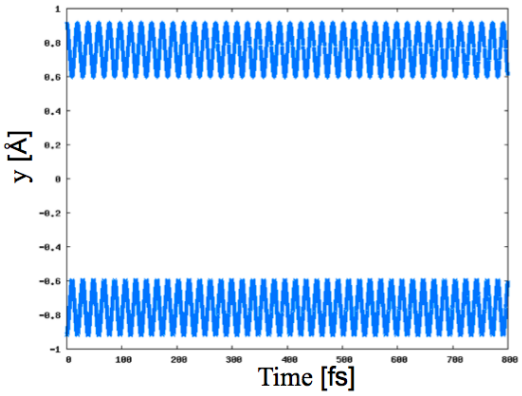


Fig.3 Temporal evolution of displacement

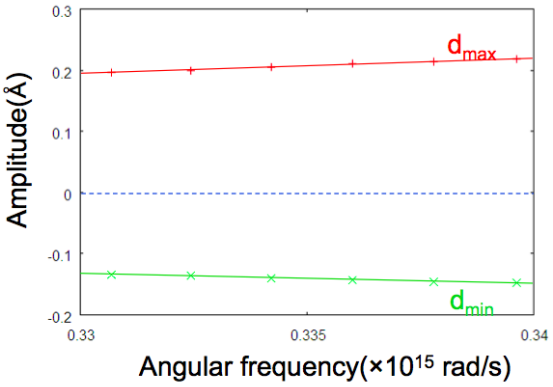
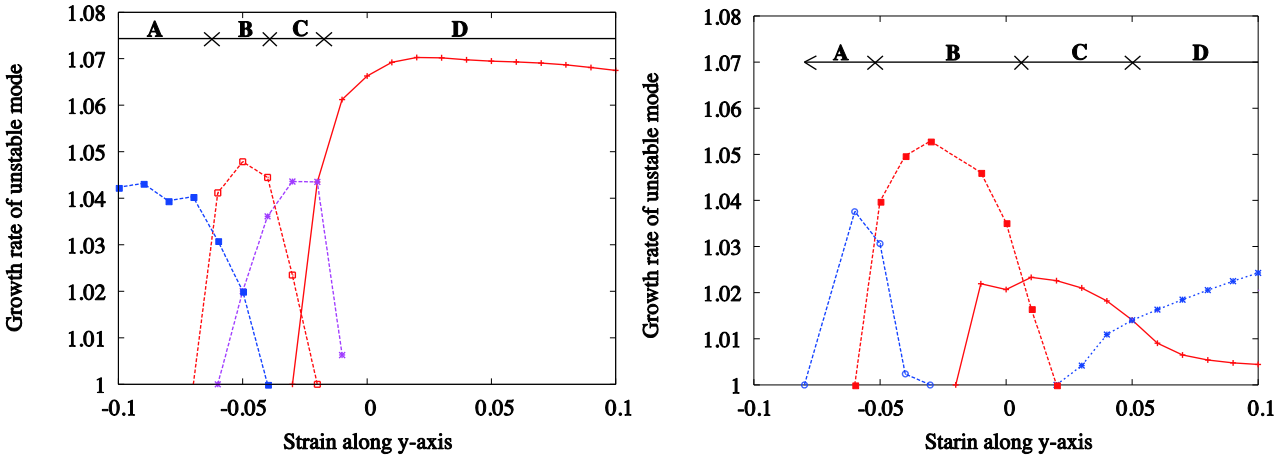
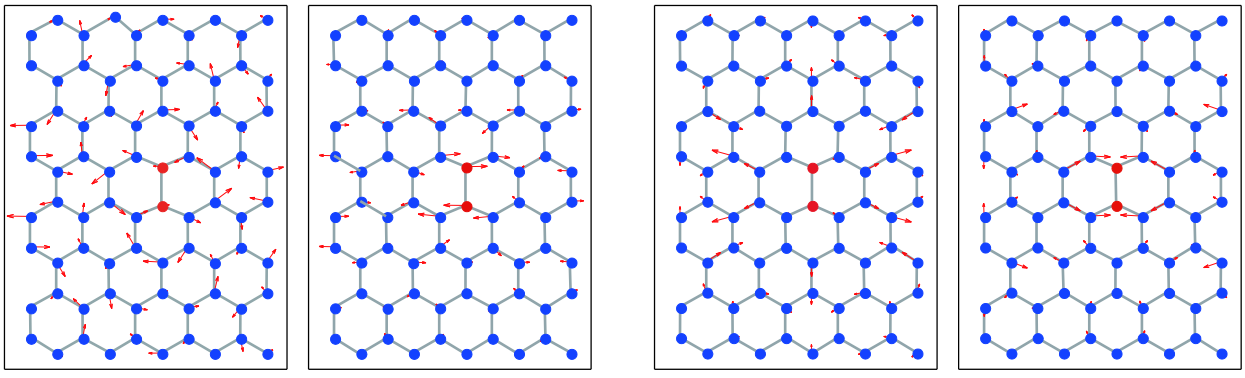


Fig.4 Relation between frequency and amplitude



(a) (b)

Fig.5 Growth ratio of unstable mode of DB: (a)period of DB T = 19ps, (b) T = 19.5ps.



(a) (b)

Fig.6 Displacement of unstable perturbation mode with maximum growth ratio: (a)T=19ps, (b)T=19.5ps.

Stability of the DB is an important feature for the study of dynamics. We investigate linear stability of the numerical precise solution of DB by solving the eigenvalue problem of Floquet matrix of DB. Floquet matrix can be constructed by calculating temporal evolution of the variational equations around the DB solution. This can be also performed by the molecular dynamic simulations. We show the result of stability analysis under applying uniaxial strain to

graphene. Figure 5 shows the growth rate of unstable perturbation mode around the DB. Complex change of the growth rate against the strength of strain is observed. Some unstable modes appear and disappear as the strain changes. Behavior of the growth rate also depends on the period of DB. We find two types of typical behavior. In one case, the maximum growth rate appears in the case of the positive strain shown in Fig. 5(a). Another case, the maximum growth rate appears in the case of negative strain shown in Fig. 5(b). Instability of DB means that the DB with perturbation or external force collapse and emit energy to the surrounding atoms. Stability analysis gives the information of displacement of the unstable perturbation modes. Figure 6 shows the displacement of the unstable perturbation modes with the maximum growth rate of the above-mentioned two typical cases. Red colored atoms indicate the position of DB. In both cases, it is found that unstable motion is excited around the atoms at which the DB is excited. In the right figure of Fig.6(a), shear motion of atoms is observed, which is perpendicular to the DB's vibration and localized on the DB's position. In the right figure of Fig.6 (b), unstable displacement is also localized on the position of DB. There results suggest that if the DB is excited in the crystals, their instability process leads to rearrangement of atoms because the DB has large energy than the phonon modes. Recently, Shimada *et al* has reported very interesting result of the molecular dynamic simulation, in which atomic structure of carbon nanotube changes due to excitation of DBs [8]. Our results suggest that the starting point of change of crystal structure due to DB.

4. CONCLUSION

We investigate the DB excited in graphene as nonlinear energy vibration modes in crystals. We successfully obtain precise numerical solutions of DB in graphene. Using these solutions, the linear stability of DB in graphene is also investigated. Some unstable perturbation modes with the maximum growth rate are also localized around the DBs. Therefore displacement pattern of the unstable perturbation modes can become a trigger of change of structure of atom using energy of the DB.

ACKOWLEADGMENT

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