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Numerical Study on Intrinsic Localized Modes in Carbon Nanotubes with Bending and Torsion

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Abstract—In this paper, structures and dynamics of Intrinsic Localized Modes (ILMs) in carbon nanotubes (CNTs) are investigated by molecular dynamics (MD) simulation. Systematic study of ILM with various deformations such as bending, torsion, and tensile deformation is performed. Moreover, lifetime of ILMs is astimated by numerical results of MD simulation.

1. Introduction

Recently, ILM attracts the attention of researchers as vibration at atom-scale in materials. Especially, some analyses has been made about the effect of tensile deformation on ILM in graphene nanoribbon and carbon nanotube [1–3]. However, the influence of other deformation such as torsion and bending on ILM is not yet clarified completely. In this research, we aim to investigate the characteristics of ILM with respect to introducing various initial deformation condition using the model of CNT.

2. Model

As shown in Figure 1, the structure of CNT is uniquely determined by chiral vector $\overrightarrow{C_h}$.

$$\overrightarrow{C_h} = m\overrightarrow{\alpha_1} + n\overrightarrow{\alpha_2} \tag{1}$$

Empirical potential proposed by Brenner [4] is used as interaction.Torsion of CNTs is introduced by rotating the top layer of CNT about $\pi/6$ to the bottom layer.Then structure optimization is performed with fixing the top and bottom layers in all directions.Numerical integrations is performed by the velocity Verlet method with time step $\Delta t = 1.0 \times 10^{-14}$s.

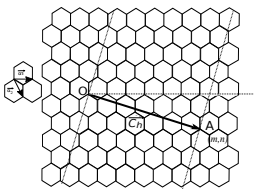

Figure 1: Schematic illustration explaining chiral vector.

3. Results and Discussion

In Figure 2, particle energy distribution and vibration of atoms in z-axis are shown. It is shown that with initial torsion, ILM is excited. Lifetime and other characteristics will be investigated in the future work.

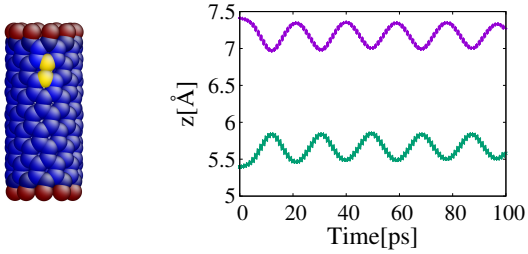

Figure 2: ILM in (10,0) zigzag CNT with torsion:(left)particle energy distribution, (right) vibration of atoms in z-axis.

Acknowledgments

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