論 文 の 内 容 の 要 旨

論文題目　Modeling of thermally induced vibration of carbon nanotubes

（カーボンナノチューブの熱励起振動のモデリング）

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In this thesis, the motion of SWNT caused by its thermal energy is focused to count the similarity with continuum mechanical transverse motion of quasi-1D molecular system. The amplitude of transverse mode from the free thermal vibration of cantilevered SWNT in Molecular Dynamics (MD) simulation have shown a good agreement with Gibbs-Botzmann distribution when the potential energy of transverse modes is simplified into harmonic continuum bar models in a plane. [1] In this study, it is revealed that SWNT vibration with its thermal energy has highly nonlinear regime. When the motion of SWNT is observed in time domain using Poincare map, two kinds of the motion, the planar and non-planar motion are periodically appeared during the whole simulation time with various aspect ratio of SWNT and several temperature conditions. While the motions are exchanging each other, the rotation direction of non-planar motion is found to be also opposed from one and another, for instance, from clock-size rotation to counter-clock wise or vice versa.

The nonlinear behavior of thermal-mechanical motion of SWNT is compared with the analytic solution of the nonlinear beam model, in which the bending along the two independent coordinates is considered at the same time using strain tensor. [2] Since the given solution of the nonlinear beam equation is derived for suspended transverse mode using Galerkin method, the solution for cantilevered fixation is newly derived with longer wave vector for cantilevered motion, and is realized that the solution has the same expression with the suspended case, but the parameter used during the derivation has slightly different physical interpretation.

Cantilevered motion in various length of SWNT using MD simulation is compared with the analytic solution and the 3 unknown parameters are found as the result of fitting. Among those, only one parameter is fully adjusted freely to match the motion and rotation exchange of motion, and shows strong tendency with the aspect ratio of SWNTs. The same tendency to suspended SWNT is found in MD simulation result and the empirical formulation is offered as the result of painstaking fitting. The fitted results show good agreement in frequency range with multiple peaks for 1st transverse mode.

The multiple resonance peaks has been reported in Field Effect Transistor (FET) experiments where the suspended SWNT is excited electromechanically with the frequency near its resonance frequency. [3,4] The parameters provided from the empirical formulation show the same number of peaks and shape in frequency range. From good agreements in simulation and experiment, it is concluded the nonlinear equation of motion from strain energy is capable of describing the mode coupling in macroscopic motion of molecules, which is dependent on temperature, aspect ratio and the rigidity of the boundary conditions.

The solution of free vibration of SWNT, therefore, gives new viewpoint that such multiple peaks are its natural characteristics, not its nonlinear response from the forced excitement. The relaxation process for 1st transverse mode, which have known as the reason of peak broadening

in continuum mechanics should be reconsidered as the result of the energy exchange between transverse modes in two orthogonal planes in case of quasi-1D molecular system.

The analytic solution derived from 1^{st}-1^{st} normal mode coupling explains other characteristics such as; 1) frequency shift dependent on the total amplitdue, 2) periodic motion exchange between non-planar and planar motion, 3) rotational direction exchange of non-planar motion. While the motion is changing its rotational direction, however, it is not always remained as predicted with the solution, this is supposed due to the mode interaction limited only to 1^{st}-1^{st} mode. Normal mode energy transfer between other modes should be included for the accuracy.

This achievement shows the continuum mechanical approach can explain the molecular motion even with the relaxation time condition in free vibration cases, whose measure is Q factor. The causality of such peak broadening or multiple peaks are explained with its nonlinearity of mechanical motion not thermal noise. The involved parameters in analytic solution show strong tendency on temperature and aspect ratio of tubes.

The reason why Green Lagrange strain can be a common feature linking continuum mechanics and molecular systems, is mainly due to the entanglement by the anharmonicity, which makes the bending in one plane coupled with orthogonal vibrations. Theoretically, phase velocity of elastic wave should not varied by the magnitude of wave vector, but the nonlinear mechanical motion due to the anharmonicity of structure allows such condition.

The solution for suspended boundary condition also corresponds well with the experimental result under the external forced excitation. This implies the multiple resonance appearance in force excitation cases can be the direct causality of the natural frequency response firstly and then, the deformed by nonlinear damping later. The frequency response from free vibration, having same peaks with forced condition means that the damping process might not

be the main cause, but the response of forced excitation has to be multiple peaks because the vibration energy at 1st mode is contained with mode coupling as producing beating signal which is composed of several peaks.

From the good agreement with the nonlinear continuum bar theory, modifying the coarse grained molecular dynamics (CGMD) with thermally induced motion of SWNT is challenged as adapting the Green-Lagrangian strain energy model into CGMD algorithm. The motion of CGMD using strain energy instead of simple spring constant shows whirling motion which is not found in conventional CGMD simulation. The detailed characteristics such as motion exchange or rotation exchange do not reached by replacing the length spring algorithm.

Lastly, the role of the smallest wave length to the response of SWNT during various external excitation is studied, which is out of range of continuum mechanical regime. The mechanical collision from other tubes, forced mechanical excitation with resonance frequency and thermally disturbed boundary condition is analyzed using Normal Mode Decomposition (NMD). As the result, the mode with small wave length has influential role to the damping of the motion in long wave length, 1st transverse mode.

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