Nonlinear Thermal Vibration of Typical Nanostructures

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Abstract. The thermal induced vibration of typical low dimensional nanostructures is investigated by using molecular dynamics (MD) simulation and the continuums models. The nonlinear dynamics equations for vibrations of the typical nanostructures are established, with the geometric nonlinearity of the large deformation taken into account. The thermal vibration of nanostructures is predicted by numerically integrating of the dynamic equations of the nonlinear beam and plate models via the-fourth-order-Runge-Kutta algorithm. The Root of Mean Squared (RMS) amplitudes and the stationary probability densities of the thermal vibration of the nanostructures are obtained via MD simulations and the continuum models. In addition, the effects of van der Waals force on the nonlinear thermal vibration of nanostructure are also investigated.

Introduction

Thermodynamic behaviours of nanostructures are very important to understanding the properties of the next generation of thermoelectric, nanoelectronic and photovoltaic devices. Carbon nanotubes (CNTs) and single-layer black phosphorus sheet (SLBP) have attracted much research interest for their excellent properties and widely potential applications. The thermal vibration of nanostructures, which is crucial to their application as a mechanical resonator, has stimulated a large number of researches. It is well known that nonlinearity may play an important role in the thermal and electrical transport of nanowires, nanotubes, nanoribbons and nanofilms. High temperatures lead to large-amplitude thermal vibration, along with geometric nonlinearity, which will have a significant effect on the thermal vibration behaviours of nanostructures. Very recently, the thermally induced free nonlinear vibration of single-walled CNTs (SWCNTs) was investigated. A cubic relationship between the displacement and the load has been observed in SLBPs under large deflections by nanoindentation experiments. The effects of the thermal stimulation on the nonlinear vibrational behaviour of CNTs and SLBPs would be very interesting. Therefore, it is necessary to reveal nonlinear dynamics behaviors of CNTs and SLBPs with thermal excitation.

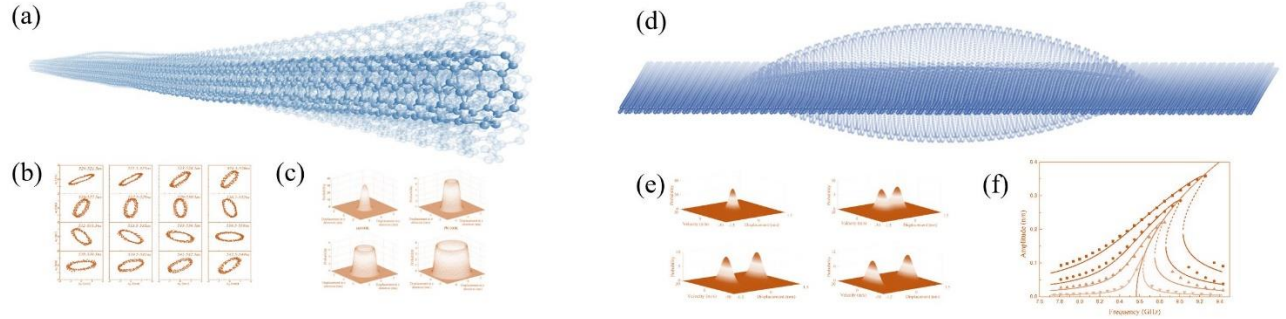

Figure 1. Nonlinear thermal vibration of typical nanostructures. (a) Snapshots of nonlinear thermal vibration of a SWCNT simulated by molecular dynamics. (b) Tip trajectories of nonlinear thermal vibration of a SWCNT. (c) The joint probability density of thermal vibration displacement components of a SWCNT. (d) Snapshots of nonlinear forced vibration of a SLBP simulated by molecular dynamics. (e) The joint probability density of displacement and velocity of thermal vibration of a SLBP. (f) Forced nonlinear vibration amplitude of a SLBP versus excitation frequency under different harmonic excitation forces.

Results and discussion

The dynamic behaviors of nanostructures excited by the thermal motion of atoms are investigated using an molecular dynamics (MD) method under canonical ensemble or microcanonical ensemble cases. The amplitude of nanostructures at thermal equilibrium was predicted by beam and plate models together with the law of energy equipartition and MD. Energy transfer between flexural motions of nanostructures due to coupling between flexural modes caused by the geometric nonlinearity of nanostructues is found. Nonlinear beam models and plate models are built to describe the nonlinear dynamic behaviors of nanstructures. Some results are presented in Figure1. In addition, the effects of van der Waals force between layers of two dimensional nanostructures on the nonlinear thermal vibration are also investigated. The present work should be of great help for designing NEMS resonators based on typical nanostructures.

References

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