 ICCES, vol.11, no.3, pp.65-65

Thermal effect on the vibrational behaviors of single-walled carbon nanotubes using molecular dynamics and modified molecular structure mechanics

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Summary

This study attempts to explore the thermal effect on the vibrational behaviors of single-walled carbon nanotube (SWCNT) using both a constant temperature molecular dynamics (MD) simulation that incorporates a Nosé-Hoover thermostat and a modified molecular structure mechanics (MMSM) model. The MD simulation is combined with a Nosé-Hoover thermostat, which controls the temperature of the system by an additional thermal reservoir. On the other hand, the MMSM model adopts equivalent beam elements and spring elements to simulate the bonding and non-bonding interactions between atoms, respectively, where the effect of temperatures can be also taken into account through Badger's rules.

The natural frequencies of SWCNTs at different temperatures, and also the Young's modulus, are calculated by those two approaches. The tendencies of the results obtained from those two approaches are quite consistent, demonstrating the validity of the present approaches. Results show that the natural frequencies and the Young's moduli of SWCNTs decrease with the increase of temperature, which agree well with the results in literatures. In addition, it also turns out that the thermal effect on natural frequencies of SWCNTs is not remarkable at low temperatures (300∼800K).

In conclusion, this study provides a well understanding of the vibrational behaviors of SWCNTs at different temperatures, including natural frequencies and their corresponding mode shapes, and also the temperature effect on the associated Young's modulus. Moreover, those two approaches presented can be further adopted to accurately explore the thermal effect on other mechanical properties of nanomaterials.

keywords: Single-Walled Carbon Nanotubes, Molecular Dynamics, Nosé-Hoover Thermostat, Modified Molecular Structure Mechanics, Thermal Effect; Vibrational Behaviors, Young's Modulus.

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