LETTER

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A novel dual–signal output screwing oscillator based on carbon@MoS$_2$ nanotubes

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Abstract: In this letter, a new CNT@MST screwing nano-oscillator is presented to investigate the coupling effect of screwing motion on inner-tube oscillation behavior via the classical MD method. The proposed oscillator is also compared with the traditional DWCNT screwing oscillators. In our simulations, the second-generation reactive empirical bond-order (REBO) potential is used to account for the intratubal atomic interactions of CNTs, while the atomic interactions of MSTs are calculated using the Stillinger–Weber (SW) potential, which has been successfully used to study the mechanical behavior of MoS$_2$ by Refs. 18, 30, 31. In recent years, there have been a few studies on the potential of MoS$_2$,$^{18,32–38}$ Based on the SW potential developed by Ref. 18, the mechanical properties of MoS$_2$/graphene heterostructures,$^{33}$ the buckling of single-layer MoS$_2$ under uniaxial compression,$^{34}$ and the phonon modes in MSTs$^{35}$ have been investigated. Based on the REBO potential developed by Ref. 30, Ref. 36 simulated the mechanical behavior of MSTs under compression, tension and torsion. Reference 37 reviewed most of the available force fields for MoS$_2$, focusing on the calculation of the properties involved in determining tribological behavior. From that work, recommendations for a proper choice of empirical potentials to use in a computational study were provided. Reference 38 evaluated the accuracy of the mechanical properties of monolayer MoS$_2$ using the MD method with the CVFF1, CVFF2, SW and REBO potentials and found that in the case of large deformation, the SW potential developed by Ref. 18 is more accurate than the other potentials, although the CVFF2 and REBO potentials can predict well the elastic properties of monolayer MoS$_2$ in the case of small deformation.$^{25,26}$

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Carbon nanotubes (CNTs),$^1$ one type of nanoscale carbon material with a special form of circular tubes, have wide applications in nano electromechanical systems (NEMS) due to their excellent electrical, mechanical, chemical and optical properties.$^{2,3}$ As a consequence, designing nano-oscillators based on double-walled CNTs (DWCNTs) or multi-walled CNTs (MWCNTs) has become an important task in NEMS technology studies. During the past decade, lots of efforts$^{4–14}$ have been devoted to the investigation of the oscillation behaviors of single–signal output nano-oscillators by applying an initial axial translational excitation or a rotational excitation to the inner tube, but no study on dual–signal output screwing oscillators has been reported so far.

In some transition metal sulfides having two-dimensional molecular structures,$^{15,16}$ such as molybdenum disulfide (MoS$_2$) and wolfram disulfide (WS$_2$), tubular structures similar to CNTs can also be formed.$^{17}$ Reference 18 found that a single-layer MoS$_2$ sheet has a higher quality factor than graphene. In addition, MoS$_2$ can be used in NEMS for designing electronic devices such as field emission sensors,$^{19}$ biosensors,$^{20}$ and memory chips.$^{21}$ Reference 22 studied the nanomechanical properties of MoS$_2$ nanotubes (MSTs) via nanoindentation and compression experiments. MSTs have good compatibility with CNTs due to the excellent physical and chemical properties of MSTs and their high similarity in structure to CNTs.$^{23,24}$ As a result, CNT@MSTs have great potential applications in multifunctional engineering systems.$^{25,26}$

Recently, Ref. 27 established a CNT@MST oscillator model by means of the molecular dynamics (MD) method to study the effects of intertube spacing and chirality on the oscillation behavior of the inner tube, indicating that the oscillation effect of a CNT@MST oscillator is superior to that of a DWCNT oscillator. Reference 28 simulated rotating self-excited DWCNT oscillators by the MD method, and pointed out that a rotating self-excited oscillator can oscillate at frequencies above gigahertz, but the amplitude of the self-excited axial oscillation is small (less than 0.5 nm) and unstable, which significantly limits its application prospects. It can be expected that two signals can be output by simultaneously applying an axial translational excitation and a rotational excitation to the inner tube. However, no report on the coupling effect of screwing motion on the oscillation behavior of CNT@MST screwing oscillators has been made so far.

In this letter, a new CNT@MST screwing nano-oscillator is presented to investigate the coupling effect of screwing motion on inner-tube oscillation behavior via the classical MD method. The proposed oscillator is also compared with the traditional DWCNT screwing oscillators. In our simulations, the second-generation reactive empirical bond-order (REBO) potential is used to account for the intratubal atomic interactions of CNTs, while the atomic interactions of MSTs are calculated using the Stillinger–Weber (SW) potential, which has been successfully used to study the mechanical behavior of MoS$_2$ by Refs. 18, 30, 31. In recent years, there have been a few studies on the potential of MoS$_2$,$^{18,32–38}$ Based on the SW potential developed by Ref. 18, the mechanical properties of MoS$_2$/graphene heterostructures,$^{33}$ the buckling of single-layer MoS$_2$ under uniaxial compression,$^{34}$ and the phonon modes in MSTs$^{35}$ have been investigated. Based on the REBO potential developed by Ref. 30, Ref. 36 simulated the mechanical behavior of MSTs under compression, tension and torsion. Reference 37 reviewed most of the available force fields for MoS$_2$, focusing on the calculation of the properties involved in determining tribological behavior. From that work, recommendations for a proper choice of empirical potentials to use in a computational study were provided. Reference 38 evaluated the accuracy of the mechanical properties of monolayer MoS$_2$ using the MD method with the CVFF1, CVFF2, SW and REBO potentials and found that in the case of large deformation, the SW potential developed by Ref. 18 is more accurate than the other potentials, although the CVFF2 and REBO potentials can predict well the elastic properties of monolayer MoS$_2$ in the case of small deformation.$^{25,26}$
and the CNT is applied with an initial separation distance of 2 nm and an initial rotational frequency of 200 GHz. The length of the inner and outer tubes is around 6 nm and 4 nm, respectively.

At the beginning, the two tubes in each mode have a symmetrical layout along the axis, where the centers of both the inner and outer tubes along the axial direction are maintained at the same position. The whole system is put in a heat bath at a temperature around 0.001 K for 20 ps after energy minimization, which allows the system to fully converge at the specified temperature after the energy minimization, where the number of particles, volume and absolute temperature of the system are constant (called the canonical NVT ensemble, where $N$ is the total number of particles, $V$ is the volume of the system and $T$ is the absolute temperature). Then, pull the inner tube outward for 20 ps at a velocity of 0.1 nm ps$^{-1}$ under constant temperature. After 20 ps (the initial separation distance of the inner tube is 2 nm), the inner tube is released from this velocity restraint and applied with a rotational excitation at a frequency of 200 GHz for 20 ps. As our simulations show that the influence of the duration of the rotational excitation on the oscillation behavior can be ignored, here the duration of the rotational excitation is set to be 20 ps in all simulations. Thereafter, we remove the rotational excitation of the inner tube and the whole system varies under constant energy conditions, where the number of atoms, volume, and energy of the system remain constant (called the microcanonical NVE ensemble, where $N$ is the same as given above and $E$ is the total energy in the system). LAMMPS$^{11}$ (Large-scale Atomic/Molecular Massively Parallel Simulator) is employed in the simulation with an analysis step size of 1 fs and an NVE total simulation time of 2 ns.

We define the intertube spacing $\alpha$ as the distance between the inner S atoms in the MST and the C atoms in the CNT, as shown in Fig. 1(b). According to Ref. 23, the equilibrium distance between a CNT and an MST is approximately 0.44 nm. Reference 6 reported that the equilibrium distance between inner and outer tubes in an MWCNT is around 0.34 nm. Here we construct CNT(9,9)@MST(14,14), CNT(9,9)@CNT(14,14) and CNT(18,0)@CNT(27,0) screwing oscillators with the intertube spacing $\alpha$ close to the respective equilibrium distance and compare their oscillation behaviors, in which the $\alpha$ of the CNT(9,9)@MST(14,14), CNT(9,9)@CNT(14,14) and CNT(18,0)@CNT(27,0) screwing oscillators are 0.447 nm, 0.329 nm and 0.356 nm, respectively. The evolution of the positions of the mass centers of the inner tubes (MCITs) and the rotational frequencies of the inner tubes (RFITs) for the CNT@MST and CNT@CNT screwing oscillators is plotted in Fig. 2. It can be seen from Fig. 2(a) that, for the CNT@MST oscillator, the axial oscillation amplitudes hardly decay, whereas for the CNT@CNT oscillators, the oscillation amplitudes dissipate more severely, which indicates that the oscillation behavior of the CNT@MST screwing oscillator is more stable than that of the CNT@CNT screwing oscillators. Figure 2(b) plots the evolution of the RFITs for the CNT@MST and CNT@CNT screwing oscillators with time, indicating that for the CNT@MST screwing oscillator, the dissipation of the rotational frequency is very small and the inner tube can perform a stable rotation at the initial frequency of 200 GHz, whereas for the CNT@CNT screwing oscillators, the rotational frequency decays sharply with time. The reason is that compared with the traditional CNT@CNT oscillators, the MST in the CNT@MST oscillator has a three-layer structure and a lower frictional coefficient.$^{20}$ Figure 2 provides evidence that the traditional CNT@CNT screwing oscillators have significant dissipation in both oscillation amplitude and rotational frequency during the screwing oscillation process, while the CNT@MST screwing oscillator can oscillate axially with an almost equal oscillation amplitude and rotate circumferentially with the initial rotational frequency, indicating that CNT@MST is more suitable as a potential candidate for a stable and low-loss screwing oscillator than CNT@CNT.

In order to investigate the effect of $\alpha$ on the oscillation behavior of the CNT@MST screwing oscillator, four CNT@MST screwing oscillator models with different $\alpha$ are considered: CNT(6,6)@MST(24,0), CNT(9,9)@MST(24,0), CNT(10,10)@MST(24,0) and CNT(12,12)@MST(24,0), whose $\alpha$ are 0.653 nm, 0.440 nm, 0.382 nm and 0.246 nm, respectively. The CNT(9,9)@MST(24,0) oscillator with an equilibrium distance of 0.440 nm exhibits an almost equal amplitude oscillation and equal frequency rotation during the
screwing oscillation process. As shown in Fig. 3, oscillators with larger \( \alpha \) have more severe off-axial rocking motion than those with smaller \( \alpha \). For example, the CNT(6,6)@MST (24,0) oscillator has the largest \( \alpha \) among the four oscillators, so its inner tube performs an off-axial rocking motion with the largest displacement, which is about over 100 times that of the other three oscillators. The frictional effect between the inner and outer tubes is closely related to the off-axial rocking motion. From Fig. 4 it can be seen that \( \alpha \) significantly affects the inner tube’s dissipation rate of both oscillation amplitude and rotational frequency: as \( \alpha \) is far from the equilibrium distance, the dissipation of both oscillation amplitude and rotational frequency is more severe. This is mainly because when \( \alpha \) is smaller than the equilibrium distance, a decrease in \( \alpha \) may enhance intertube interaction, which causes the frictional effect between tubes to rise sharply and results in an increasingly pronounced dissipation behavior of the inner tube during the screwing oscillation. In contrast, when \( \alpha \) is greater than the equilibrium...
distance, an increase in $\alpha$ may cause the off-axial rocking motion distance to rise and then enhance the friction effect.

To further investigate the effect of $\alpha$ on the dissipation rate of the axial translation oscillation amplitude and the rotational frequency of the inner tubes for both CNT@MST and CNT@CNT during screwing motion, the offset of $\alpha$ is defined as $\lambda = \alpha - \alpha_0$, in which $\alpha_0$ is the equilibrium distance. It should be noted that for the CNT@MST models, $\alpha_0 = 0.44$ nm, while for the CNT@CNT models, $\alpha_0 = 0.34$ nm. Dimensionless dissipation rates $\lambda = \frac{\Delta A}{\Delta t\bar{c}}$ and $\varpi = \frac{\Delta \omega}{\Delta \omega_0}$ are defined to describe the dissipation rates of the axial oscillation amplitude and the circumferential rotational frequency, respectively. $\Delta A$ and $\Delta \omega$ are the dissipation of the oscillation amplitude and the rotational frequency in the whole simulation respectively, $n$ is the total number of cycles in the simulation, the initial separation distance $A_0 = 2$ nm and the initial rotational frequency $\omega_0 = 200$ GHz.

The variations of $\lambda$ and $\varpi$ for the CNT@MST and CNT@CNT screwing oscillators with respect to $\lambda$ are plotted in Figs. 4(a) and 4(b), respectively, from which it can be seen that their values are very small when $\lambda$ is near zero and they are increased when $\lambda$ is far from zero. We assume that the screwing oscillation is unstable when $\lambda$ or $\varpi$ rises sharply as $\lambda$ is far from zero, as shown in Fig. 4. The figure indicates that the CNT@MST screwing oscillators have a wider adjustable $\alpha$ than the CNT@CNT screwing oscillators. It can also be seen that the dissipation rates of both the axial oscillation amplitude and rotational frequency of the CNT@MST screwing oscillators are lower than those of the CNT@CNT screwing oscillators during screwing oscillation. References 6, 10, 42 also reported that CNT@CNT oscillators perform stable and sustained oscillation when $\alpha$ is about 0.34 nm. We also find that a stable and low-loss screwing oscillation can be obtained based on CNT@MST heterogeneous nanotubes in a wider range of spacing values from 0.289 to 0.653 nm, indicating a stronger advantage over oscillators that are based on traditional CNT@CNT nanotubes, which exhibit stable, sustained and low-loss screwing oscillation only when $\alpha$ is 0.340 to 0.376 nm.

In summary, we have presented a novel CNT@MST screwing oscillator that can provide outputs of both rotational and oscillatory signals simultaneously. The effect of intertube spacing on oscillation behavior is especially investigated. The MD method results show that, compared with the traditional double-walled carbon nanotube (CNT@CNT) screwing oscillators, CNT@MST screwing oscillators have three obvious advantages: better stability, lower energy dissipation rates, and wider adjustable intertube spacing.

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Fig. 4. (Color online) Dimensionless dissipation rates (a) $\lambda$ and (b) $\varpi$ with respect to the offset $\lambda$ of the intertube spacing.
38) S. Xiong and G. X. Cao, Nanotechnology 26, 185705 (2015).